GE Healthcare
Life Sciences

UNICORN™ 5.31

User Reference Manual

Chapter 1 to 11

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1 Introducing UNICORN

Introduction

This chapter contains:

- A general overview of the UNICORN system.
- Information about the user documentation for UNICORN and how to use it.

In this chapter

This chapter contains these sections.

Section	See page
1.1 About UNICORN	10
1.2 About this manual	14
1.3 About the UNICORN user documentation	17

1.1 About UNICORN

Introduction

This section is a general overview of the UNICORN system.

What is UNICORN?

UNICORN 5.31 is a complete package for control and supervision of liquid chromatography, cross flow filtration or oligonucleotide synthesis systems. It consists of control software and a controller card or unit for interfacing the controlling PC to the liquid handling module.

Liquid chromatography is used in separation processes, for analytical purposes or in the biochemical process industry.

UNICORN is a trademark of GE Healthcare.

Operating environment

UNICORN 5.31 runs on a PC using the following operating systems:

- Microsoft™ Windows™ XP Professional (32-bit)
- Microsoft Windows 7 Professional (32-bit)
- Microsoft Windows 7 Professional (64-bit)

It is designed to run under English keyboard settings.

Note: UNICORN version 5.30 is compatible with 32-bit operating system versions only.

Windows functions

Most Windows functions are also available in UNICORN, including

- cut and paste
- right-click short-cut menus

Note: Drag and drop is not available. File and folder handling in UNICORN also differ from the general Windows file manager standard.

Bar code reader

You can connect a bar code reader to the PC and use the reader to enter information instead of using the keyboard. This can be useful for example when entering information like batch IDs.

Compatible systems

UNICORN can be used with a number of chromatography systems including

- ÄKTA™ design systems
- OligoProcess™ systems
- BioProcess™ systems

Note: All examples in this guide are based on an ÄKTAexplorer™ 100 system that operates with the E100F400 strategy. If you use another system you may find that the descriptions and instructions do not match your system on every point. In that case you also need to refer to the user documentation for your specific chromatography system.

System networks

UNICORN can be installed on a stand-alone computer to control only a single, locally attached system. However, a stand-alone computer can control up to four separate systems. In a network installation each computer workstation can operate many systems regardless if they are locally connected or not. Each system can only be operated by one workstation at a time, but several may view the output data.

Software modules

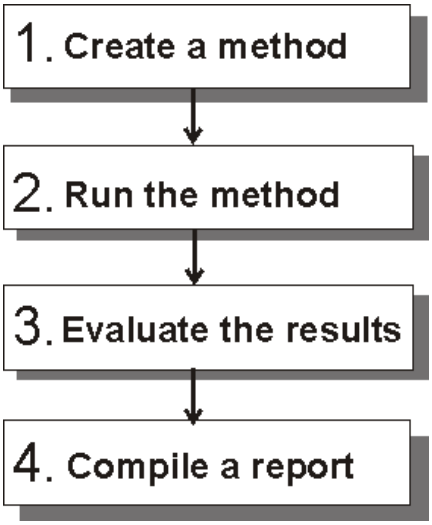
The UNICORN control software consists of four integrated modules:

Module	Function
UNICORN Manager	File handling and administration, e.g. definition of systems and user profile etc.
Method Editor	To create and edit methods for pre-programmed control of chromatography systems.
System Control	To control and monitor the separation processes online, through method-based or manual control.
Evaluation	To evaluate and present stored results from separation processes.

Note: All modules are active when the program is operating, and are not closed when they are minimized. A minimized System Control unit may control a process. All modules will normally open when the program is started. However, a user profile may be set up so that not all modules are available. Only the available modules will be displayed.

Work flow

The work flow in UNICORN can be divided into four distinct stages. Each stage is described in separate chapters in this manual. The flow chart below shows the work flow stages.



Help functions

An online help utility is included in the UNICORN software. The table below describes how to access the help utility.

If you want to access...	Then...
the general help utility.	open the ***Help*** menu in any of the software modules.
context-specific help topics.	• click the ***Help*** button in the dialog box or • press the **F1** key on your keyboard.
the online manuals.	open the ***Help*** menu in any of the software modules and select ***Manuals***.

Security

The table below describes the main security functions in UNICORN:

Feature	Function
Access Security	Only authorized users can access UNICORN. Each user is assigned an access level, which defines the functions that the user is permitted to use.
Connection Security	A running system can only be controlled from one connection. Systems may be locked with a password to prevent other, unauthorized users from changing parameters.
Data Security	Result files from an ongoing run can be saved automatically at preset intervals to minimize data loss if the system fails. The results are saved locally if the network communication fails.
Electronic Signatures	Method and result files can be signed electronically for enhanced security and accountability.

1.2 About this manual

Introduction

This section is a general description of the manual, the contents and the pre-requisites for the examples and instructions that are presented in the User Reference Manual.

The purpose of the User Reference Manual

The purpose of the User Reference Manual is to present a comprehensive guide to the UNICORN system for a user either with previous experience of this system or from other, similar chromatography systems. The system is presented in detail, along with practical instructions of how to operate a model system.

Systems covered by this manual

This manual and the corresponding version of Getting Started with UNICORN covers the following systems:

- ÄKTAexplorer
- ÄKTApurifier™
- ÄKTAFPLC™
- ÄKTAbasic™
- ÄKTApilot™
- Ettan™ LC

Note: Adapted versions of this manual are available for ÄKTAxpress™, ÄKTA oligopilot™ and BioProcess™ systems.

The model system

UNICORN software can be used in numerous possible system variations. For practical reasons the user documentation is based on a model system that consists of:

- ***ÄKTAexplorer 100***
- Strategy ***E100F400***
- ***Frac-950***

Note: If you use another system you may find that the descriptions and instructions do not match your system on every point. In that case you also need to refer to the user documentation for your specific chromatography system.

Refer to other manuals

The User Reference Manual does not contain information about the installation procedure or network configuration. You will find this information in the Administration and Technical Manual.

Sometimes you may find it more convenient to refer to the Getting Started with UNICORN guide for a linear, step-by-step instruction how to perform a task.

Document structure

The manual is divided into chapters. Each chapter starts with a brief overview that presents the contents and the headings for the sections that the chapter contains. Most sections begin with an introduction that summarizes the content. Some sections are divided into sub-sections.

A section is divided into blocks of information with separating lines. The blocks are identified by a label in the margin. This makes it easier for you to quickly scan a page to find the exact topic you are looking for.

Typographical representations

Menu commands, field names and other text items from the software are quoted exactly as they appear on the screen, in a bold italic typeface:

Example: ***Run Setup***

Search paths are shown in a bold italic typeface with a separating colon between each level:

Example: ***View:Panes:Customize*** (i.e. the menu command ***Customize*** in the sub-menu ***Panes*** from the ***View***-menu).

Text entries that UNICORN generates or that the user must type is represented by a monotype typeface:

Example: `Connection change`

Prerequisites

The following prerequisites must be fulfilled before you can use this manual the way it was intended:

- You need to have a general understanding of how your PC and Windows works. In most cases universal computer functions will not be explained.
- UNICORN must be installed and configured correctly on your computer.
- You need to understand the concepts of liquid chromatography. Terminology and functionalities will be explained only when they differ from normal practise.
- Before you try to operate a chromatography based on the instructions in this manual you need to study and understand the safety information that is part of the system documentation.

1.3 About the UNICORN user documentation

Introduction

The user documentation for UNICORN 5.31 is divided into three separate manuals.

This section is an overview of the contents and the relationship between the manuals.

The manuals

The three UNICORN 5.31 manuals are:

- Getting Started with UNICORN 5.31
- UNICORN 5.31 User Reference Manual (See *Section 1.2 About this manual, on page 14*).
- UNICORN 5.31 Administration and Technical Manual

Information about UNICORN 5.31 is also included in the manuals for the ÄKTAexplorer systems, that is

- ÄKTAexplorer User Manual
- ÄKTAexplorer, ÄKTApurifier and ÄKTAmicro Operating Instructions

User info about Getting Started with UNICORN 5.31

The questions and answers in the table below describe the features of the Getting Started with UNICORN 5.31 manual.

Question	Answer
Who should read Getting Started with UNICORN 5.31?	Users that are new to the UNICORN system and with limited experience from other systems.
What do I need before I start?	A basic knowledge of PC and Windows functions and an understanding of the concepts and terminology of liquid chromatography.
What are the contents of Getting Started with UNICORN 5.31?	Basic descriptions of UNICORN and its use, based on a model system.
How should I use Getting Started with UNICORN 5.31?	Read in front of your computer and test the instructions at the same time.

User info about the UNICORN 5.31 User Reference Manual

The questions and answers in the table below describes the features of the UNICORN 5.31 User Reference Manual.

Question	Answer
Who should read the UNICORN 5.31 User Reference Manual?	• Users that are experienced with previous UNICORN system versions. • Users with vast experience from other systems.
What do I need before I start?	Knowledge of PC and Windows functions and an understanding of the concepts and terminology of liquid chromatography. Preferably previous experience with UNICORN.
What are the contents of the UNICORN 5.31 User Reference Manual?	• Detailed descriptions of UNICORN 5.31. • Instructions on how to use the software, with suggested alternatives. Most instructions are based on a model system.
How should I use the UNICORN 5.31 User Reference Manual?	Depending on your previous experience you can either read whole chapters from the beginning to the end, or only selected sections for reference.

User info about UNICORN 5.31 Administration and Technical Manual

The questions and answers in the table below describes the features of the UNICORN 5.31 Administration and Technical Manual.

Question	Answer
Who should read the UNICORN 5.31 Administration and Technical Manual?	System administrators.

Question	Answer
What do I need before I start?	• General knowledge of UNICORN. • Knowledge of PC, Windows and general network administration functions. • An understanding of the concepts and terminology of liquid chromatography.
What are the contents of the UNICORN 5.31 Administration and Technical Manual?	Detailed instructions of: • How to install and maintain UNICORN in a network environment. • How to create and administrate user profiles. Most instructions are based on a model system.
How should I use the UNICORN 5.31 Administration and Technical Manual?	• If you are an experienced administrator of previous UNICORN versions you can read selected sections for reference. • If this is your first experience of UNICORN we recommend that you study the manual in detail.

2 UNICORN concepts

Introduction

This chapter contains:

- Definitions and descriptions of some of the specific concepts that are presented in this manual and in other UNICORN manuals.
- An overview of the UNICORN user interface.
- A Quick Start Guide that can be used as a shortcut for experienced users that want to start right away.

Note: General concepts and common terminology are not explained here.

In this chapter

This chapter contains these sections.

Section	See page
2.1 Concept definitions	21
2.2 The UNICORN user interface	25
2.3 Quick Start Guide	54

2.1 Concept definitions

Introduction

This chapter contains explanations and definitions of a number of UNICORN concepts that are used in this manual.

The concepts are organized in alphabetical order.

Alarms

Systems settings or method instructions specify acceptable limits for monitor signals during a run. An ***Alarm*** dialog box will be displayed on the screen if the monitored values exceed or fall below specified limits. The system will be paused.

Batch run

You can perform a ***Batch run*** of a number of result files in the ***Evaluation*** module. The files do not have to be open and the run operates in the background. The procedure is useful if you want to print a number of results with the same settings, or if you want to perform integration with the same parameter settings on many results.

BufferPrep

BufferPrep is a function to prepare a buffer of different pH and salt concentrations online from four stock solutions. This eliminates the need to manually prepare new buffers every time the pH needs to be changed.

Note: ***BufferPrep*** is only available for some ÄKTAdesign systems.

Chromatogram

A chromatogram is a collection of data represented by a number of curves that have been created during a run, including UV, conductivity, pH, fraction marks etc. The original raw data curves cannot be deleted or modified. They can be used as a basis for evaluation procedures and subsequent creation of new curves.

A chromatogram can also contain curves that have been created and saved during an evaluation session.

Curves

The monitor signals from the run are displayed graphically as curves.

Note: Log text entries and similar events from the run are treated as curve data in UNICORN even though they are not shown graphically as curves in the chromatogram.

Method

The program instructions for a run are defined in a ***Method***. A Method can be divided into blocks that represent steps in the separation process. Each block consists of a series of instructions that request specific operations in the system.

MethodQueue

MethodQueues are used to link several methods together, on the same or on different systems.

Example: A ***MethodQueue*** can be set up to conduct a CIP study of a number of columns, through a controlled series of scouting runs.

Method Wizard

The ***Method Wizard*** is a user-friendly tool to create new methods. The ***Wizard*** takes the user step-by-step through the creation process.

Method Wizards are supplied with UNICORN installations for ÄKTAdesign systems.

Result files

UNICORN creates ***Result files*** when a method is run. The ***Result files*** contain:

- Run data from the monitors in the system.

  Example: UV absorbance, flow rate, conductivity etc.

- Documentation from the run.

  Example: Logbook entries, calibration settings, scouting parameters, text method etc.

- Saved results from evaluations of the run data.

  Example: Peak integrations, simulated peak fractionations etc.

Scouting

Scouting is used to repeat a series of ***Method runs*** automatically with predetermined changes in the values for one or more ***Variables***. A ***Scouting Scheme*** is defined as part of the method.

Scouting is used for optimizing chromatographic processes.

Strategy

Part of the UNICORN software is specific for the system that it is set up to operate. The system specific part is usually referred to as the ***Strategy***. The ***Strategy*** defines available method and manual instructions, system settings, run data, curves and Method Wizards.

Note: The examples in this guide are generally based on the ***E100F400*** strategy.

Template

Templates are basic methods that can be used as a starting point for developing customized methods. The method variables in a suitable ***Template*** is adjusted to create a method for another application.

Variable

Instruction parameters and values at breakpoints in the ***Method*** may be defined as ***Variables***. ***Variables*** makes it easy to adapt a method to a particular run.

- A framework ***Method*** with default parameters can be changed to create variants.
- A ***Method*** can be used in automatic ***Method Scouting***, where one or more parameter ***Variables*** are changed systematically.

Warnings

Systems settings or method instructions specify acceptable limits for monitor signals during a run. A ***Warning*** dialog box may be displayed on the screen if a specified limit is exceeded. The system will still continue to run after a ***Warning***.

2.2 The UNICORN user interface

Introduction

This section is an overview of the four UNICORN modules with descriptions of some of the elements of the user interface. The section also contains a description of the search functions in UNICORN.

Note: A user profile can be set up so that the user only has limited access to the modules described in this chapter. Only the available modules will open when the program is started.

In this section

This section contains these sub-sections.

Section	See page
2.2.1 UNICORN Manager	26
2.2.2 The Method Editor module	30
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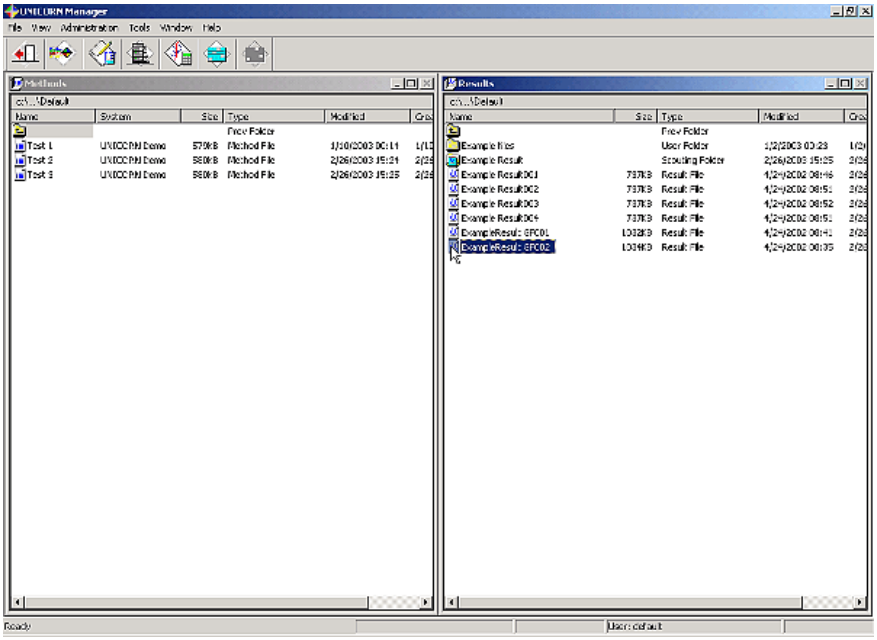
2.2.1 UNICORN Manager

Introduction

The ***UNICORN Manager*** is mainly used for file and folder administration.

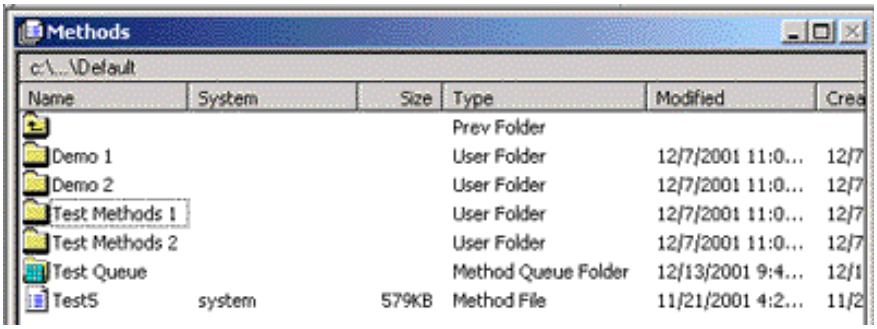
The UNICORN Manager windows

The module is divided into two windows, the ***Methods*** window and the ***Results*** window. See the illustration below:



The Methods window

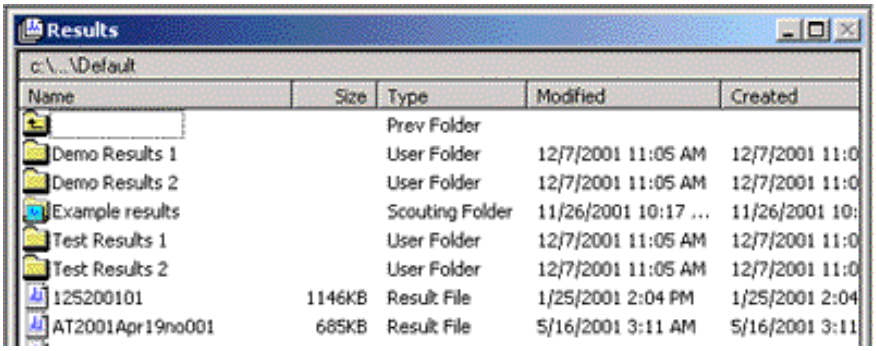
The ***Methods*** window contains all the saved methods, ***MethodQueues*** and all the folders containing methods that are available to the user. See the illustration below:



Note: The icons for ***MethodQueue*** folders are different from the regular folder icon.

The Results window

The ***Results*** window contains all the saved results and all the result folders.



Note: The icons for ***Scouting*** folders are different from the regular folder icon.

Toolbar icons in the UNICORN Manager

The table below describes the toolbar icons in the module.

Icon	Function
	The ***Logon/Logoff*** icon is used to log on or log off the system. **Note:** The arrow in the ***Logoff*** icon points away from the door.
	The ***Instant Run*** icon immediately starts a run from a selected template or from a wizard.
	The ***New Method*** icon opens the ***Method Editor*** module and displays the ***New Method*** dialog box.
	The ***System Control*** icon activates the first connected ***System Control*** module and displays the ***Manual instruction*** dialog box. **Note:** If no ***System Control*** module is connected, a module will be activated and the ***System Connect*** dialog will be displayed.
	The ***Evaluation*** icon opens the ***Open Result*** dialog box. Select a result file and click ***OK*** to start the ***Evaluation*** module.
	The ***MethodQueue*** icon opens the ***MethodQueue Editor***.
	The ***Existing MethodQueue*** icon opens the ***Running MethodQueue*** dialog box to display ***MethodQueues*** in progress.

Limited access to the UNICORN Manager

Some user groups may be defined to have only a limited access to the ***UNICORN Manager*** functions. The available functions in the limited version are:

- ***Log off***
- ***Change User Attributes***
- ***Change Password***
- ***Quit Program***
- ***Help***

There is also a ***Cancel*** button which minimizes the dialog box. The illustration below shows the limited access version of the ***UNICORN Manager***.

Note: For more information about how to change passwords and user attributes please refer to *Section 3.4 How to change your passwords and user attributes, on page 69*. For more information about how to log off and quit the program, please refer to *Section 3.1 Log on routines and log off routines, on page 56*.

2.2.2 The Method Editor module

Introduction

The ***Method Editor*** module provides complete facilities for advanced editing of the methods.

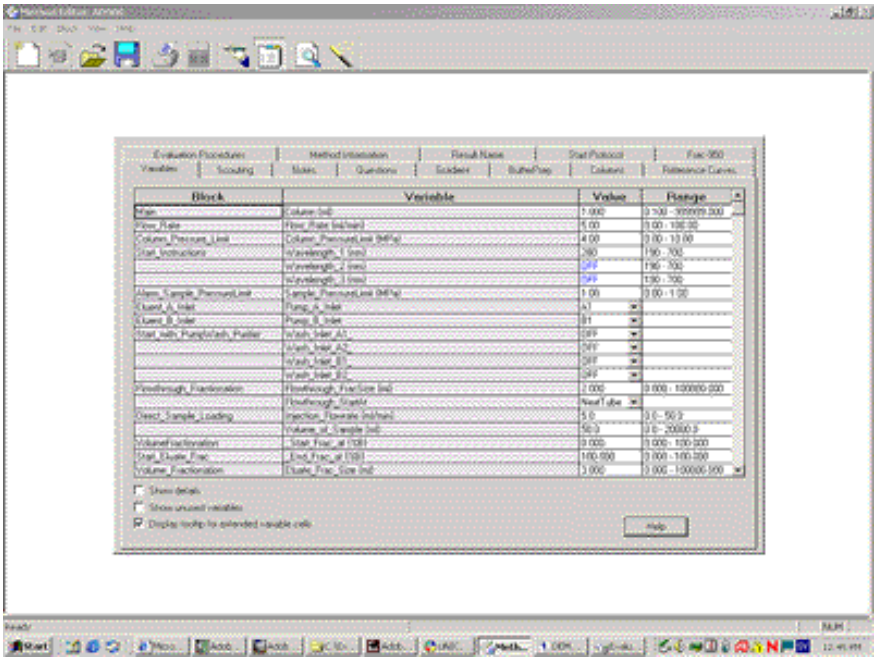
Two modes

The ***Method Editor*** interface operates in two modes:

- ***Run Setup***
- ***Text Instructions***

Run Setup

Run Setup is a dialog box with a number of tabs that define the method properties. See the illustration below:

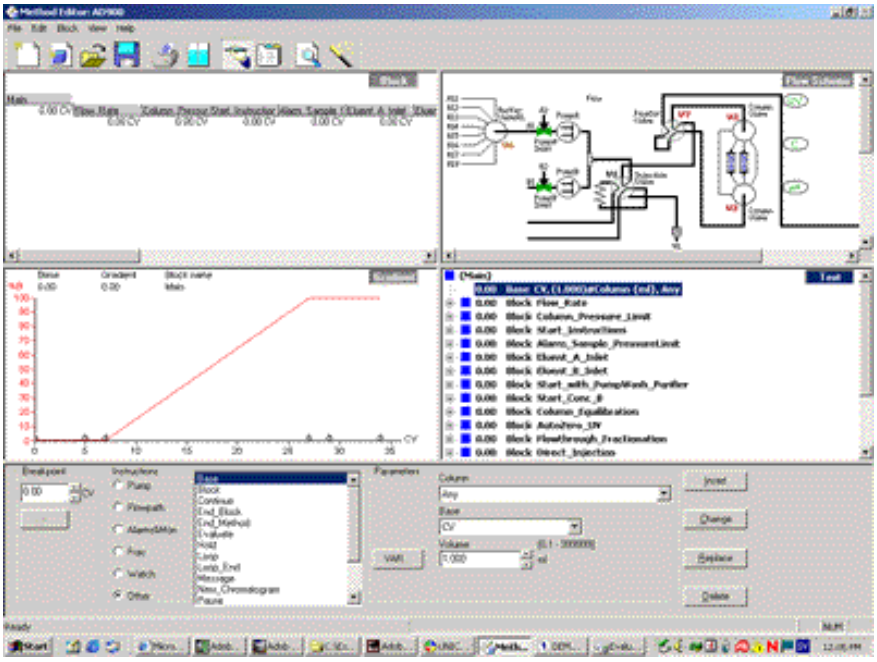


Text Instructions

Text Instructions are used for advanced editing. Up to five different display panes can be open at the same time:

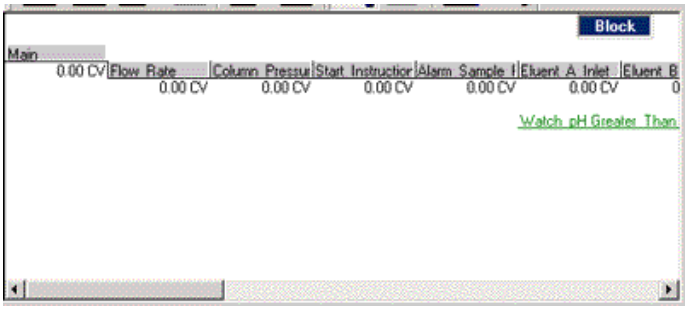
- The ***Block*** pane.
- The ***Flow Scheme*** pane.
- The ***Gradient*** pane.
- The ***Text*** pane.
- The ***Instruction box*** pane.

See the illustration below:



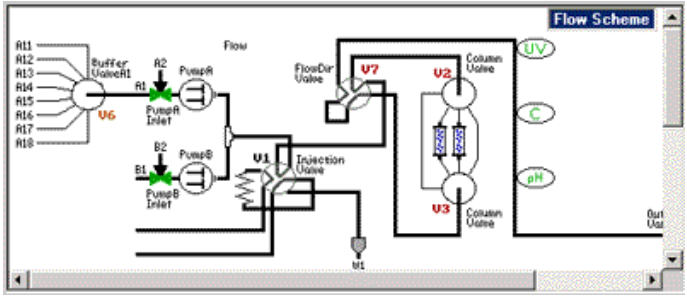
The Block pane

The ***Block*** pane contains a graphical representation of the method organized in blocks. See the illustration below:



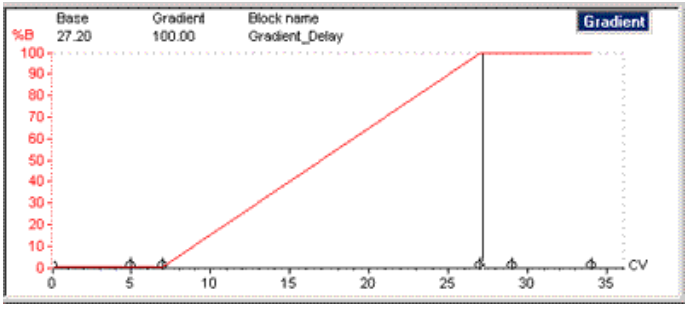
The Flow Scheme pane

The ***Flow Scheme*** pane displays the configuration of the system components. The pane is static and for information only. See the illustration below:



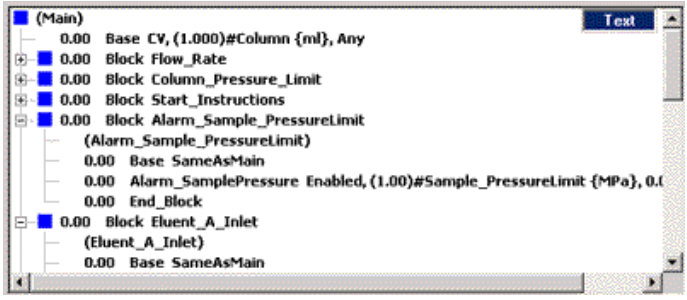
The Gradient pane

The ***Gradient*** pane provides a graphical overview of the block structure and eluent gradient in the current method. See the illustration below:



The Text pane

The ***Text*** pane displays the method as a list of text instructions. The instructions can be organized in blocks, denoted by blue square symbols. The blocks can be expanded to show the instructions within the block. See the illustration below:



The Instruction box pane

The ***Instruction box*** pane is used to enter, edit or delete instructions. See the illustration below:

Toolbar icons in the Method Editor

The table below describes the toolbar icons in the module.

Icon	Function
	The ***New*** icon opens the ***New Method*** dialog box. The dialog box is used to create a new method.
	The ***New Block*** icon opens the ***New Block*** dialog box, which is used to add blocks to a method.
	The ***Open*** icon displays all available method files and method folders in the ***Open*** dialog box.
	The ***Save Method*** icon saves the edited method.
	The ***Print*** icon opens the ***Print*** dialog box. Select the method elements that you want to print.

Icon	Function
	The ***Customise Panes*** icon opens the ***Customise Panes*** dialog box, which is used to select the panes that are open in ***Text Instructions*** mode.
	The ***Text Instructions*** icon opens the ***Method Editor*** in ***Text Instructions*** mode.
	The ***Run Setup*** icon opens the ***Method Editor*** in ***Run Setup*** mode.
	The ***Log Format*** icon opens the ***Log Format*** dialog box, which is used to display the accumulated time or volume for a method.
	The ***Method Wizard*** icon opens the ***Method Wizard***, which is used to create new methods.

2.2.3 The System Control module

Introduction

The ***System Control*** module is used to perform and monitor runs.

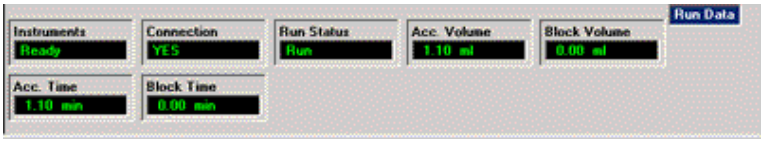
The System Control panes

The ***System Control*** module contains four different display panes that can be opened all at once or in any combination:

- The ***Run Data*** pane.
- The ***Curves*** pane.
- The ***Flow Scheme*** pane.
- The ***Logbook*** pane.

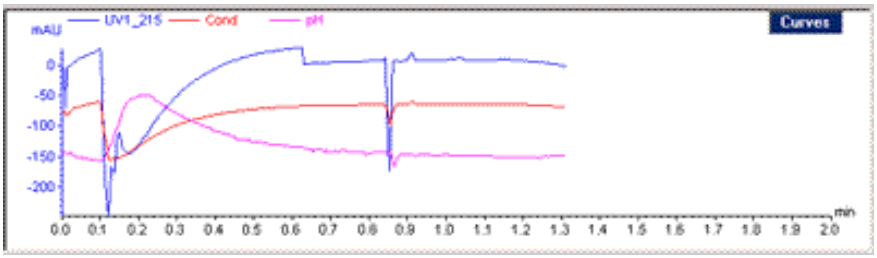
The Run Data pane

The ***Run Data*** pane displays the current values for the selected run parameters. The values are updated at regular intervals, which are defined in the system strategy. See the illustration below:



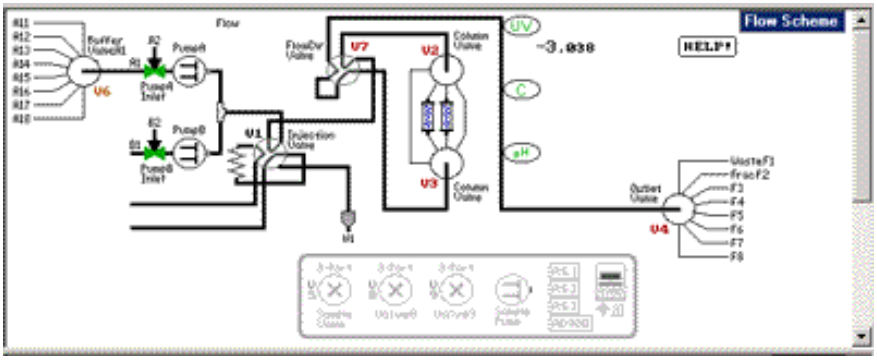
The Curves pane

The ***Curves*** pane displays monitor signal values graphically. See the illustration below:



The Flow Scheme pane

The ***Flow Scheme*** is a graphical representation of the chromatography system. During a run, the ***Flow Scheme*** displays open flow paths in color. Monitor signals can be displayed numerically. See the illustration below:

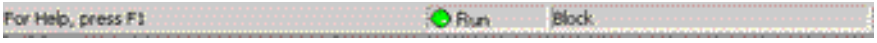


The Logbook pane

The ***Logbook*** pane displays all actions during a separation run, e.g. method start and end, base instruction, method instructions and manual instructions such as ***Pause*** or ***Hold***. See the illustration below:

The Status bar

The ***Status bar*** in the bottom of the ***System Control*** module displays the current status of the separation run. See the illustration below:



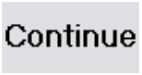
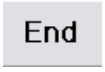
The current system status is represented by the colored dot:

- A green dot represents a running system.
- A red dot represents a system in ***Pause*** state.
- A yellow dot represents a system in a ***Hold*** state.
- A white dot represents a system in an ***End*** state.

Toolbar icons in the System Control

The table below describes the toolbar icons in the module:

Icon	Function
Run	The ***Run*** icon opens the ***Run*** dialog box, which shows all available methods. If a method is loaded, ***Run Setup*** opens.

Icon	Function
	The ***Hold*** icon suspends execution of the method, while liquid is still pumped at the current flow rate and eluent concentration.
	The function of the ***Pause*** icon depends on the strategy. The ***Pause*** icon suspends execution of the method and stops all pumps so that the system comes to a standstill.
	The ***Continue*** icon resumes the execution of a paused or held method.
	The ***End*** icon terminates the method execution and puts the system into an ***End*** state.
	The ***Customize Panes*** icon opens the ***Customize Panes*** dialog box, which is used to select the display panes that are open.
	The ***View Documentation*** icon opens the documentation pages. Run notes can be entered in the ***Notes*** page and settings can be changed.
	The ***View Properties*** icon opens the ***Properties*** dialog box, which is used to control the data display in the ***System Control*** panes.
	The ***Connect System*** icon is used to connect a system.
	The ***Disconnect System*** icon is used to disconnect the system.

Icon	Function
	The ***Take Control of the System*** icon is used to leave the view mode for the system and change into a control mode.
	The ***Leave Control of the System*** icon is used to leave the control mode for the system and change into a view mode.

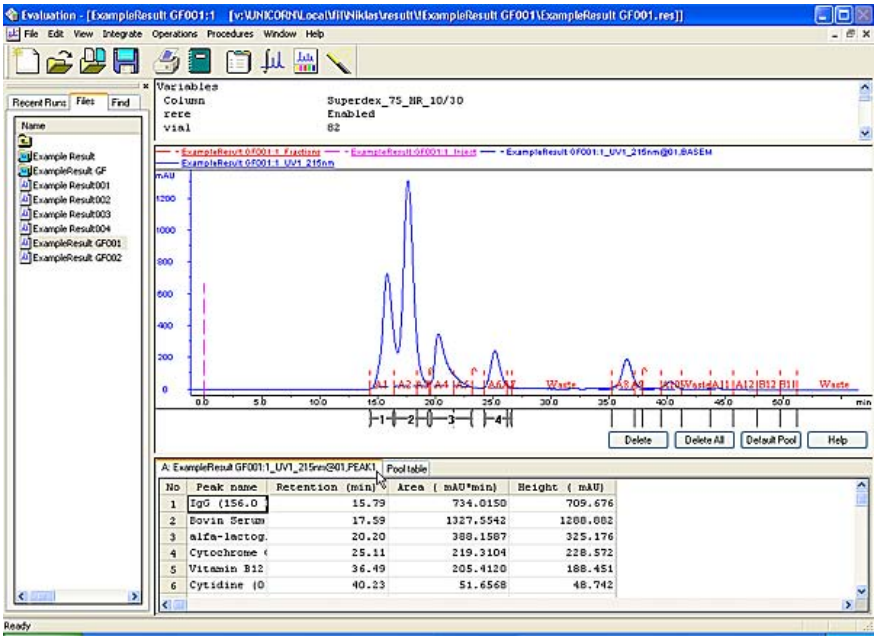
2.2.4 The Evaluation module

Introduction

The ***Evaluation*** module provides extensive facilities to present and to evaluate curve data.

The module window

Opened result files are displayed in the ***Evaluation*** module window. See the illustration below:



Toolbar icons in the Evaluation module

The table below describes the toolbar icons in the module:

Icon	Function
	The ***New*** icon opens an empty chromatogram.
	The ***Open*** icon displays all available result files and result folders in the ***Open Result*** dialog box.
	The ***Open Curves to Compare*** icon opens the ***Open Curves to Compare*** dialog box, which is used to select and open curves for comparison.
	The ***Save*** icon saves the edited result file.
	The ***Print*** icon opens the ***Print Chromatograms*** dialog box.
	The ***Report*** icon opens the ***Generate Report*** dialog box, which is used to select a report format.
	The ***View Documentation*** icon opens the ***Documentation*** dialog box, which is used to view and edit the result documentation.
	The ***Peak Integrate*** icon opens the ***Integrate*** dialog box, which is used to select peaks to integrate in a modified peak table.

Icon	Function
	The ***Chromatogram Layout*** icon opens the ***Chromatogram Layout*** dialog box, which is used to select and format curves and display items in the chromatogram.
	The ***Multifile Peak Compare*** icon opens the ***Multifile Peak Compare Wizard***, which is used to compare peak data from different result files.

2.2.5 Search functions

Introduction

This section describes the general search functions that can be used to locate for example chromatograms, curves and text strings in UNICORN. These functions can be used in several program modules, dialog boxes and wizards.

Search the Folder list

The search will take place in the displayed folder only. To select another folder, click the ***Browse*** button and open the desired folder.

Search the Result list

- The search will take place in *all* result files within the selected folder as denoted by the asterisk (*). To select specific result file(s), click the ***Browse*** button and select the result file(s).
- You can use wildcard characters to search for chromatograms within result files with a specific name profile.
  - * represents any number of characters
  - ? represents any single character

Wildcard character examples:

`iex` will search files named “iex”

`iex*` will search all files with names that begin with “iex”

`*iex` will search all files with names that end with “iex”

`?iex` will search only 4-character names that end with iex

Search the Chromatogram list

The asterisk (*) indicates that all chromatograms within a result file will be selected. Click ***Browse*** to select one or several specific chromatograms.

Search the Curve name list

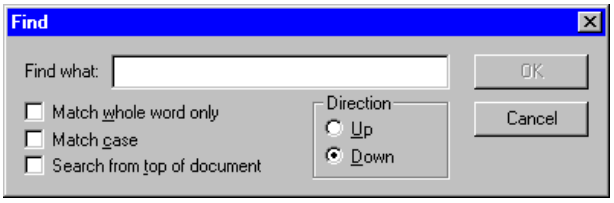
The UV curves are identified by number and sometimes wavelength. For example, UV1_280, UV2_280 and UV1_254 are all different curves. To search for all UV curves, select *UV* in the ***Curve name*** text field.

Searches for Sample ID

A ***Sample ID*** can be used as a search criteria if it has been defined as a variable. The ***Sample ID*** can be entered in searches for result files both in the ***UNICORN Manager*** and in the ***Evaluation*** module.

Find a text string

The ***Find*** command is used to search for text strings:



Field	Description
Find what	Type the text string you want to find.
Match whole word only	Select the check-box if you only want complete string matches, not partial matches.
Match case	Select the check-box if you only want matches which correspond according to upper-case and lower-case letters.
Search from top of document	Select the check-box to start the search from the top of the document, otherwise the search will start from the cursor position.
Direction	Choose whether to search upwards or downwards in the document.

Commands

Use the commands below to find more occurrences of a text string after you have found the first one:

- Press ***F3*** to search for the next occurrence of the string *or* right-click and choose ***Find next***.
- Right-click and choose ***Find previous*** to search for a previous occurrence.

General information about searches

- The default setting is to search in all result files or chromatograms.
- User-entered search filters (to a maximum of 10) will be saved in the drop-down menus for both ***Result*** and ***Chromatogram*** selections. More than one string can be used as a search delimiter (insert ";" between strings), and search filters are automatically saved and stored within user profiles.
- Click ***All*** to return to the default setting to search in all result files or chromatograms.

2.2.6 Help functions and manuals

Introduction

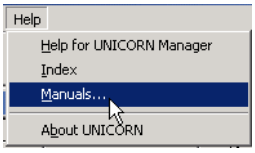
There are different ways to get help and instructions in the UNICORN application:

- From the ***Help*** menu in each module
- From the context-sensitive help in each dialog box
- By selecting the ***Online Manual*** from the ***Help*** menu
- By pressing the **F1** key
- By right-clicking an instruction in the ***Method Editor*** and selecting the ***What's This?*** menu item

The Help menu

- By choosing the ***Help*** menu item from the ***Help*** menu in each module you can access the ***Help*** file.
- By choosing the ***Manuals*** menu item from the ***Help*** menu in each module you can access the installed manuals in PDF format.

The illustration below shows the ***Help*** menu of the ***UNICORN Manager*** module:



The Help file

The table below describes how to open and use the Help file:

Step	Action
1	Choose ***Help:Index***. *Result*: The Help file is displayed with the ***Index*** panel selected.

Step	Action
2	**Search for topic in the Help Index** • Type a keyword you want help on in the text box in the panel. *Result*: The alphabetically closest matches are displayed in the list. • Select a match and click the ***Display*** button. *Result*: The associated help text is displayed in the right pane. **Search for topic using text search** • Click the ***Search*** tab • Type one or more keywords you want help on in the keyword text box. *Result*: A number of topics containing the keywords are listed. • Select a match and click the ***Display*** button. *Result*: The associated help text is displayed in the right pane.
3	• You can also click the ***Contents*** tab to view the contents of the Help file divided into sections. • Click the plus signs to expand the tree structure. • Click a topic to read the associated help text.

Manuals

When UNICORN was installed, the administrator selected which manuals to install. Therefore the available manuals may be different on your system than in the illustration below.

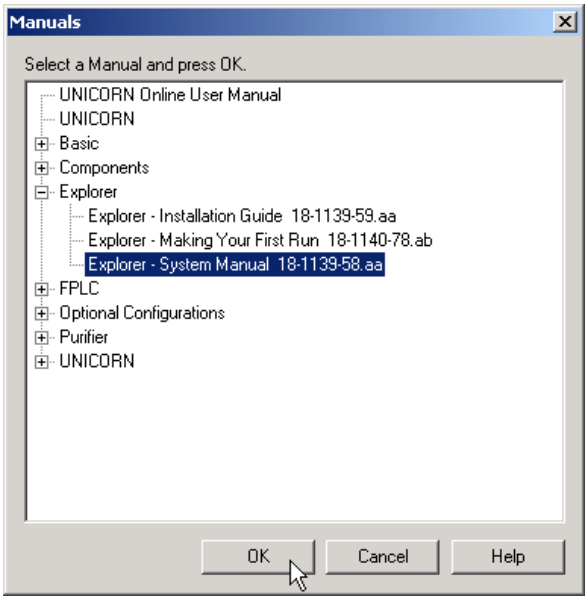
Note: Manuals can be added after the UNICORN installation. See the UNICORN 5.31 Administration and Technical Manual for more information.

How to open a manual

To open a manual

- choose ***Help:Manuals*** in the ***UNICORN Manager*** module.

Result: The ***Manuals*** dialog box is opened.



- Select the manual and click the ***OK*** button.

Note: Some manuals are only available in PDF format.

Context-sensitive help

In each dialog box there is a ***Help*** button. If you press that button, either of the following will be displayed:

- A message box with relevant information, for example the dialog box options.
- The Help file, with relevant information displayed in the right pane.

2.2.7 Snapshots

Introduction

A ***Snapshot*** provides information about a method run at a certain point in time. It contains information about the values of all the variables at the selected point.

Snapshot functionality is available in

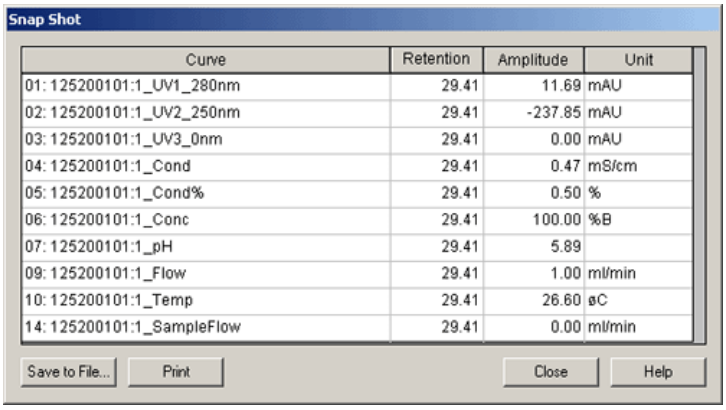
- the ***Method Editor***, where Snapshot instructions can be inserted in a method to be recorded during the method run.
- the ***System Control*** module, where you can take Snapshots during a run using the Marker.
- the ***Evaluation*** module, where you can take Snapshots from a result file using the Marker.

How to take Snapshots during a method run

The table below describes how to take Snapshots in the ***System Control*** module during a method run:

Step	Action
1	A method is running and the ***System Control*** is displayed: • Right-click in the ***Curves*** pane and select ***Marker*** in the menu. *Result*: A vertical line is displayed.
2	Click the marker line and drag it to the desired point where you want to take a Snapshot.

Step	Action
3	Right-click in the ***Curves*** pane and select ***Snapshot*** in the menu. *Result*: The Snapshot is displayed in the ***Snap Shot*** dialog box.



4

- Click the ***Save to File*** button if you want to save the information as an Excel file (***.xls***) or a tabbed text file (***.txt***).
- You can also copy the information to the clipboard:
  - Click and drag the mouse in the table to select the information you want to copy.
  - Press **CTRL**+**C**.

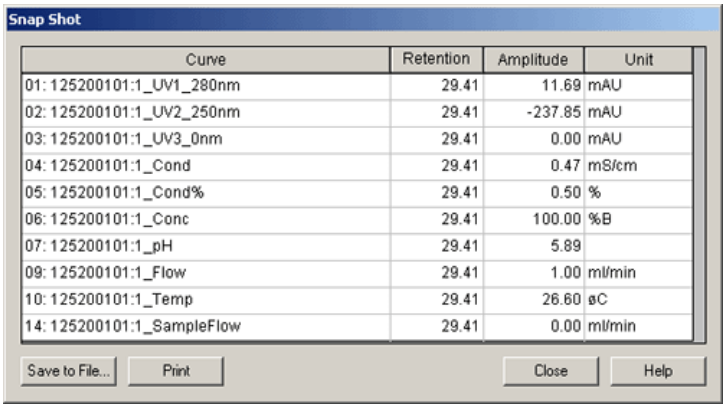
    The information can now be pasted in a text editor.
- Click the ***Print*** button if you want to print the information.
- Click the ***Close*** button.

5 Repeat steps 2 to 4 if you want to view more Snapshots.

How to take Snapshots in the Evaluation module

The table below describes how to take Snapshots in the ***Evaluation*** module:

Step	Action
1	• Open a result file in the ***Evaluation*** module. • Right-click and select ***Marker*** in the menu. *Result*: A vertical line indicating a certain point is displayed.
2	Click the marker line and drag it to the desired point where you want to take a Snapshot.
3	Right-click and select ***Snapshot*** in the menu. *Result*: The Snapshot is displayed in the ***Snap Shot*** dialog box.
4	• Click the ***Save to File*** button if you want to save the information as an Excel file (***.xls***) or a tabbed text file (***.txt***). • You can also copy the information to the clipboard: - Click and drag the mouse in the table to select the information you want to copy. - Press **CTRL**+**C**. The information can now be pasted in a text editor. • Click the ***Print*** button if you want to print the information. • Click the ***Close*** button.
5	Repeat steps 2 to 4 if you want to view more Snapshots.



How to view recorded Snapshots

The table below describes how to view Snapshots which have been recorded during a method run using the ***Snapshot*** text instruction.

Note: How to insert the ***Snapshot*** text instruction in a method is described in *Section 5.3 How to use Text instructions, on page 106*.

Step	Action
1	In the ***Evaluation*** module, • choose ***View:Documentation*** *or* • click the ***View Documentation*** icon. *Result*: the ***Documentation*** dialog box is displayed.
2	• Select the ***Result Information*** tab. • Select the ***Snapshots*** sub-tab. *Result*: The recorded Snapshot information for a chromatogram is displayed in a list.
3	You can • select other chromatograms in the ***Select chromatogram*** drop-down box. • select the ***Rows*** or ***Columns*** radio button to display each Snapshot as a row or a column. • select the ***Time*** or ***Volume*** radio button depending on which quantity you want as a base.
4	To print the Snapshot information • click the ***Print*** button • select the ***Snapshot*** check box in the ***Print*** dialog box. • click ***OK***.
5	Click ***OK*** (or the ***Cancel*** button) to exit the ***Documentation*** dialog box.

2.3 Quick Start Guide

Introduction

This guide is intended for users who are fully familiar with the safety precautions and operating instructions that are described in all manuals, i.e. experienced users of previous versions of UNICORN. The instructions assume that all installations were made according to the instructions, that the model system is used and is connected.

Quick Start instructions

The table below describes the easiest way to create a method, run the system and generate a printed chromatogram. The procedure is based on an ***Instant run***.

Step	Action
1	Click the ***Instant run*** icon in the ***UNICORN Manager*** module. *Result*: The ***Instant run*** dialog box opens.
2	• Select ***Wizard***. • Select a system (if necessary). • Click the ***Run*** button. Result: The ***Method Wizard*** opens in the ***System Control*** module.
3	Go through all selections on the ***Method Wizard*** pages. Click the ***Next*** button to proceed from page to page.
4	Click the ***Run*** button on the last page. *Result*: The start protocol opens.
5	Verify the method on the ***Variables*** page and change values as required. Click the ***Next*** button to proceed through several pages.
6	Select ***Print_Chromatogram*** in the ***Evaluation procedures*** page. *Result*: A printout will automatically be generated after the run.
7	Click the ***Start*** button on the last page. *Result*: The run starts.

3 General system operations

Introduction

This chapter describes how to start the program, assign user properties and set up the system.

Refer to the UNICORN 5.31 Administration and Technical Manual for installation and network configuration instructions.

In this chapter

This chapter contains these sections.

Section	See page
3.1 Log on routines and log off routines	56
3.2 How to create a new user	61
3.3 How to assign user properties	65
3.4 How to change your passwords and user attributes	69
3.5 How to connect to the chromatography system	72
3.6 How to back up and restore system data	78
3.7 How to set up a printer	82

3.1 Log on routines and log off routines

Introduction

This section describes how to start and quit the UNICORN program, and how to log on and log off.

Username and password

Normally the system administrator defines the users and creates your first password. The program can also be set up so you can log on without a password.

Note: The first time after UNICORN has been installed, you need to log on as a default user and create a user profile. This process is described in *Section 3.2 How to create a new user, on page 61*.

How to start the program

Note: If UNICORN is already started by a previous user, proceed to How to log on.

There are two ways to start the program:

If you start with...	Then...
a UNICORN icon on your desktop	double-click the icon
the Windows Start menu in Windows XP	locate the program under ***All programs:Unicorn*** and click the ***UNICORN*** logo
the Windows Start menu in Windows 7	locate the program under ***All programs:Unicorn*** and click the ***UNICORN*** logo

How to log on

The table below describes how to log on to UNICORN.

Step	Action
1	• Select ***Tools:Logon*** in the ***UNICORN Manager*** module *or* • Click the ***Logon/Logoff*** icon in the ***UNICORN Manager*** module *Result*: the ***Logon*** dialog box is displayed. **Note:** You do not have to perform this step if you start up UNICORN. When you start UNICORN the ***Logon*** dialog box is automatically displayed.
2	Select your username from the list.
3	Type your password (optional).
4	Click ***OK***.

The program modules

The program has four modules. When you start the program and log on you work in the ***UNICORN Manager*** module. UNICORN also automatically opens the ***Method Editor***, the ***System Control*** and the ***Evaluation*** modules. These modules are minimized until you activate them. Up to four System Control module windows may open if UNICORN was set up to control more than one system at the installation.

Note: If the access rights are limited to only some modules, the other modules will not open.

Log off after you are finished

Always log off when you leave the computer to prevent others from accidentally changing or deleting your files, or disturbing your UNICORN runs. There are two ways to log off in the ***UNICORN Manager***:

- Select ***Tools:Logoff***

or

- Click the ***Logon/Logoff*** icon.

Note: In case your access to the ***UNICORN Manager*** is restricted you will still be able to log off.

Processes can run after log off

The process will continue even if you log off while a separation run is in progress. You can leave the process locked and set a password to protect it from interference. The table below describes how to log off and set a password for a running process.

Step	Action
1	• Select ***Tools:Logoff*** in the ***UNICORN Manager*** module. *or* • Click the ***Logoff*** icon. *Result*: A confirmation box opens.
2	Click ***Yes*** to confirm that you want to log off. *Result*: The ***Leave Control of system*** dialog box opens.
3	Click the ***Locked*** radio button.
4	Type a password in the ***Password*** text box.
5	Click ***OK***.

Unlocked Log off

It is not recommended that you log off and leave a running system unlocked. This means that the run is in progress without a user that is responsible for the process.

Automated workstation lock or logout

The system administrator may set an automatic workstation lock or log off after a specified time for a user. If there are no keyboard entries or mouse movements within the time limit, the workstation will be locked or logged off.

Note: A locked workstation can be activated again only by the previous user if the regular log in password is entered. If another user wants to log on and use the workstation the previous user can be logged off without entering the correct password. The previous user's files will be closed and the new user will only have access to his own files.

Automated logout will not happen while a ***MethodQueue*** or a ***Scouting*** scheme is operating.

How to log on and unlock the system

When you log on again after leaving the system locked with a process running or after an automated workstation lock, you will be asked to unlock the system.

Step	Action
1	Log on to the system. *Result*: The ***System Unlock Confirmation*** dialog box opens.
2	Type your login password or the password that the system was locked with in the ***Password*** text box.
3	Click ***OK***

Note: You can connect in view mode only without providing the password.

Systems locked by other users

You can unlock a system that has been locked by another user if you have the correct password.

You may still be able to unlock a system even if you do not have the password. Any user with ***Unlock locked systems*** authorization can override another user's lock by entering his or her own logon password. However, it is recommended that this authorization is limited to only a few users.

How to quit UNICORN

UNICORN will still be open after you have logged off. To close the program you must log in again and quit UNICORN (you cannot quit the program if you are not logged in). The table below describes how to do this.

Step	Action
1	• Select the ***File:Quit Program*** menu command in the ***UNICORN Manager*** module. *or* • Click the close icon in the top right-hand corner of the program window. *Result*: A confirmation box opens.
2	Click ***Yes*** to confirm that you want to quit.
3	A ***Warning*** opens if you have any unsaved data in the ***Method Editor*** or ***Evaluation*** module. • Click ***Yes*** to continue to close the program. Your unsaved data will be lost when the program is closed. • Click ***No*** to return to the program and save your data.
4	The ***Leave Control of system*** dialog box opens. Select the locked or unlocked option as in the logoff procedure. **Note:** This step only happens when a system is connected.
5	Click ***OK***.

Note: Do not shut down Windows XP/Windows 7 or turn off the computer if you quit UNICORN with a separation run in progress. If you are performing a ***Scouting run*** or a ***MethodQueue run*** you cannot quit the program at all.

In case your access to the ***UNICORN Manager*** is restricted you will still be able to quit the program.

3.2 How to create a new user

Introduction

This section describes how to create a new user and assign a home folder for the user's methods and results.

Default user

A default user is created when the system is installed. The default user has unrestricted access to all UNICORN functions. You log on with this profile when you access a newly installed system for the first time.

The table below describes how to log on as the default user.

Step	Action
1	Select user ***default*** from the user drop-list.
2	Type password `default` if necessary. *Note*: The ***default*** user is the only user that is allowed to use the user name as password.
3	Click ***OK*** or press the ***Enter*** key.

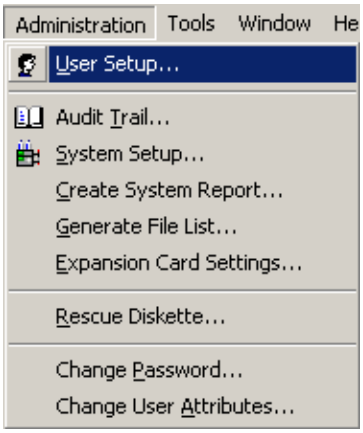
Note: We recommend that the default user is deleted when regular user profiles are created.

How to open User Setup

All user administration is performed in the ***User Setup*** dialog box in the ***UNICORN Manager*** module. It is accessible only to authorized users (and the default user).

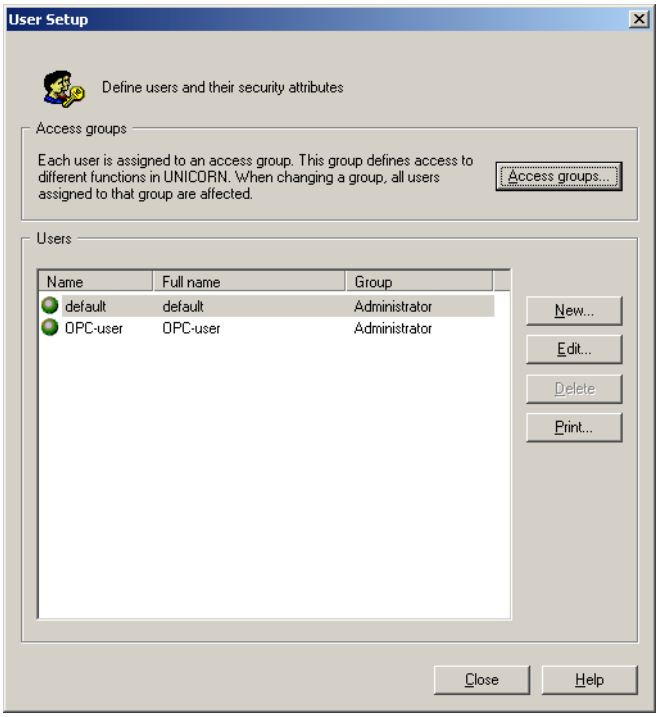
User Setup is found on the ***Administration*** menu.

- Choose ***Administration:User Setup***.



The User Setup dialog box

The illustration below shows the ***User Setup*** dialog box.



How to create a new user

The table below describes how to create a new user.

Step	Action
1	Click the ***New*** button in the ***User Setup*** dialog box. *Result*: The ***Create New User*** dialog box opens.
2	Enter a user name in the ***User name*** text box.
3	Enter the full name of the user in the ***Full name*** text box.
4	Enter the job position of the user in the ***Position*** text box.

Step	Action
5	Select or create a ***Home folder***: • Select a ***Drive*** and a folder from the ***Name*** drop-list and proceed to step 9. or • If you need to create a new home folder, proceed with step 6.
6	Click ***New***. *Result*: the ***Create New Folder*** dialog box opens.
7	Select a ***Drive*** and type a folder name.
8	Click ***OK*** to create the folder and return to the ***Create New User*** dialog box.
9	Click ***OK***. *Result*: The new user is created and added to the ***User Setup*** list.
10	• Click ***Close***. or • Click the ***New*** button and repeat steps 1 - 9 to create more users.

Home folders

Each user must be assigned to a home folder. The ***Default*** folder can be used if you do not want to assign an individual home folder.

Note: If you create a home folder on the C: (local) drive it will not be accessible from other computers. If you select a network, make sure that is addressed by the same drive letter from all computers in the network.

3.3 How to assign user properties

Introduction

A user is assigned properties that define password rules, and the folders and chromatography systems that the user can access. This section describes how to assign properties.

How to open User properties

The user properties are defined in the ***User Setup*** dialog box in the ***UNICORN Manager*** module. The table below describes how to open ***User Setup***.

Step	Action
1	Select ***Administration:User Setup***.
2	Select a user in the ***Users*** list.
3	Click the ***Edit*** button. *Result*: The ***User properties*** dialog box opens.

The ***User properties*** dialog box is used to edit the user definition and assign properties for passwords, folder and system access, and available manual instructions.

How to edit the user definition

The table below describes how to edit the user definition in the ***User properties*** dialog box.

Step	Action
1	Select the ***User*** item.
2	Select an access group from the ***Group*** drop-down box. **Note:** A pre-defined access group is assigned a certain level of access to UNICORN.
3	Select a folder from the ***Home folder*** drop-down box.
4	Click the check boxes to select ***Administrator Attributes***.
5	Click ***OK*** to finalize or select another definition to edit.

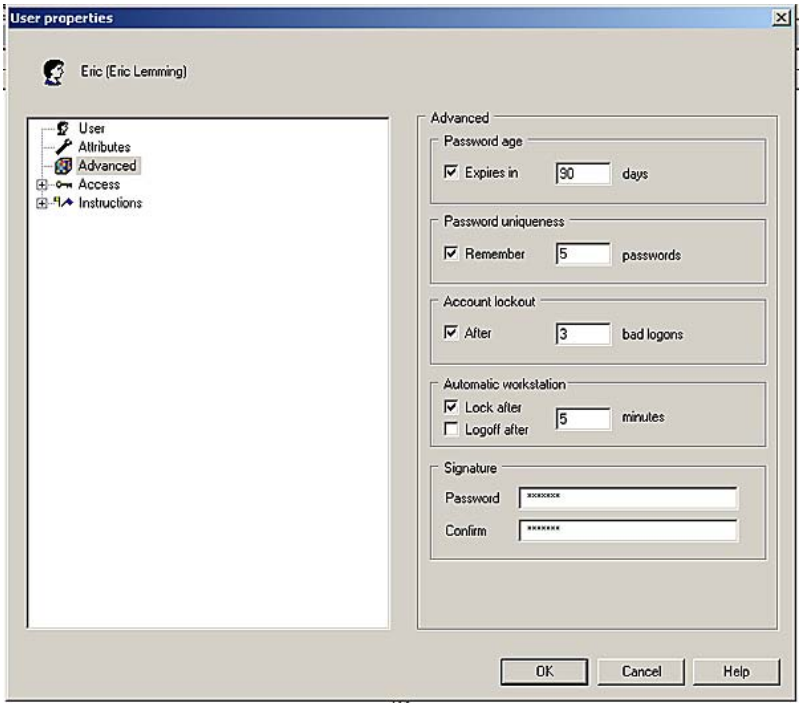
How to edit the user attributes

The table below describes how to edit the attributes in the ***User Attributes*** window pane.

Step	Action
1	Select the ***Attributes*** item.
2	Select applicable attribute items in the ***User Attributes*** pane: • Use large toolbar icons • Show unused variables • Show variable details • Default overwrite of baselines and peak tables • Prompt for column before manual runs
3	Type which curve to display in the ***Quick view*** dialog box.
4	• Select a size definition and type a value for the ***Fraction mark*** height. • Select a size definition and type a value for the ***Injection mark*** height. • Select a size definition and type a value for the ***Logbook mark*** height.
5	Click ***OK*** to finalize or select another definition to edit.

The Advanced dialog page

The ***Advanced*** window pane is used to define password policies for the user. Normally this is only used by the system administrator.



Note: This dialog page is only available if a required password was selected when the software was installed.

How to define access to folders and systems

The ***Access*** dialog page is used to define the folders and systems that the user has access to. Click the check box for each selected folder and system.

Up to 20 folders can be set up to be shared. The user has access to all files and sub-folders in the selected folders. Only selected folders will be visible in the methods or results panels of the ***UNICORN Manager*** module.

Note: All users should have access to the ***Failed*** folder on each local station in a network installation. This will ensure that users can access results that were saved in the ***Failed*** folder in case of a network communication error.

How to define available manual instructions

The ***Instructions*** dialog page is used to define the manual instructions and system sounds that are available to the user as well as which monitors the user is allowed to calibrate. Click the check box for each selected instruction, sound or monitor.

Access groups

The level of access to UNICORN functions for each user is determined by the ***Access group*** that the user is assigned to. The access authorizations can be edited for each group, normally by the systems administrator.

Refer to the UNICORN 5.31 Administration and Technical Manual if you need to edit an ***Access group***.

Note: User access can be limited to only some UNICORN modules. If that is the case the unavailable modules will not be displayed. E.g. if the ***UNICORN Manager*** is unavailable you will only have access to a dialog box with the basic functions to change limited user attributes, passwords and to log out and quit the program.

3.4 How to change your passwords and user attributes

Introduction

Every user can change his or her passwords and some user attributes even if user administration is handled exclusively by the system administrator. The changes are made in the ***UNICORN Manager***.

How to change passwords

The table below describes how to change your logon and signature passwords.

Step	Action
1	Select ***Administration:Change Password***. *Result*: The ***Change Password*** dialog box opens.
2	Type your old logon password in the ***Old*** text box. **Note:** Your passwords will only be shown as asterisks.
3	Type a new password in the ***New*** text box.
4	Repeat the new password exactly in the ***Confirm*** text box.
5	Repeat steps 2 to 4 in the ***Signature password*** section if necessary.
6	Click ***OK***.

About passwords

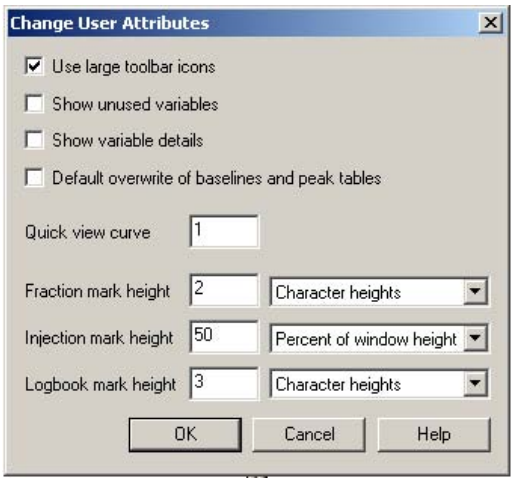
The list below is a summary of facts and advice about UNICORN passwords:

- The system can be set up to operate without required passwords.
- The minimum number of password characters is set up at installation.
- Passwords can be any combination of letters and numbers.
- Passwords are case sensitive.
- Avoid using obvious passwords, e.g. your username, your telephone number, etc.
- The settings in the ***User properties*** determine the expiration for a password. Change passwords regularly even if your user profile is set up without password expiration.

How to change user attributes

The table below describes how to change your user attributes.

Step	Action
1	Select ***Administration:Change User Attributes***. *Result*: The ***Change user attributes*** dialog box opens.



2 **Dialog check box options**

The dialog check box options are described below:

- ***Use large toolbar icons***

  Display large toolbar icons in all modules.

- ***Show unused variables***

  Show variables that are not used in the method on the ***Variable*** page of the ***Start Protocol***.

- ***Show variable details***

  Show detailed method variables on the ***Variable*** page of the ***Start Protocol***.

- ***Default overwrite of baselines and peak tables***

  When new baselines and peak tables are created, the old ones are overwritten.

Step	Action
3	**Mark heights** Select a size definition and type the height for the following marks: • Fraction mark • Injection mark • Logbook mark
4	Click ***OK***.

3.5 How to connect to the chromatography system

Introduction

A computer can have up to four chromatography systems connected at a time. This section describes how to connect to the systems, and different connection modes.

How to establish a connection

The table below describes how to connect a chromatography system that is locally connected to your computer.

Step	Action
1	Open a ***System Control*** module. *Note*: Each UNICORN installation may have up to four System Control modules. The number of modules are selected when the software is installed.
2	• Select the ***System:Connect*** menu command. *or* • Click the ***Connect to system*** toolbar icon. *Result*: The ***System Connect*** dialog box opens.
3	Select the system you want to connect.
4	Click ***OK***.

Remote connections

Each computer workstation may have up to four chromatography systems connected locally. In a network installation you may connect a system that is physically connected to another computer, the local station. Your system is then a remote station.

The local station that is connected to the chromatography system must be logged on to the network and the UNICORN drivers must be running. However, the connection will work even if the UNICORN program is not running on the local station.

Network log on

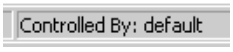
Ensure that your workstation is logged on to the network before you start a chromatography system that is directly connected to the station. You can operate a local system without logging on to the network, but there are several disadvantages to this:

- Files stored on network drives are not accessible.
- Changes made to global files, e.g. user settings files, will apply only locally and will be lost the next time you log on to the network.
- Result files that are directed to a network drive will be stored in the ***Failed*** folder on the local station.

Connection modes

Several workstations can connect to a single chromatography system at the same time but only one workstation can be in control mode. The other connections are in view mode and the connected workstations can only monitor the system activity, but not issue any commands.

The system status is indicated on the status bar at the bottom of the ***System Control*** window. The table below describes the different connection modes, the corresponding status texts and some of the various actions you can take to change the connection mode.

Connection mode	Status Text	Possible action to change connection mode
Not connected		Connect to a system.
Control mode.		Disconnect from or leave control of the system. (The system is controlled by you.)
View mode		No connection possible. (The system is controlled by another user.)
View mode		Click the ***Connect to system*** icon and supply a password. (The system is locked by another user.)
View mode		Connect to the system. (The system has been left unlocked.)

How to leave control of a system

The table below describes how to leave control of a system so that it is available to be controlled by other users.

Step	Action
1	• Select ***System:Leave Control***. *or* • Click the ***Leave control of system*** icon. *Result*: ***The Leave Control of system*** dialog box opens.
2	Click the radio buttons to select to leave the system unlocked or locked.
3	Enter a password (if the system is to be locked).
4	Click ***OK***.

How to disconnect a system

The table below describes how to disconnect from a system.

Step	Action
1	• Select ***System:Disconnect***. *or* • Click the ***Disconnect from system*** icon.

Step	Action
2	*Result*: If the system is in view mode • the system is disconnected. If the system is in control mode • the ***Leave Control of System*** dialog box opens.
3	Select to leave the system locked or unlocked.
4	Click ***OK***. *Result*: The system is disconnected.

How to disconnect when quitting

When you log off or quit from UNICORN you automatically disconnect all connected systems. A ***Leave Control of System*** dialog box will be opened for each system that was connected.

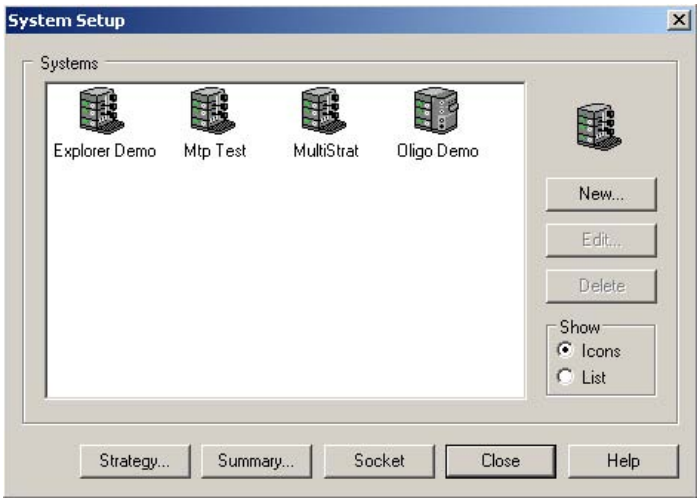
Note: If you disconnect from a system in control mode and re-connect to it, you may be connected in view mode. Another user may have taken control in the meantime.

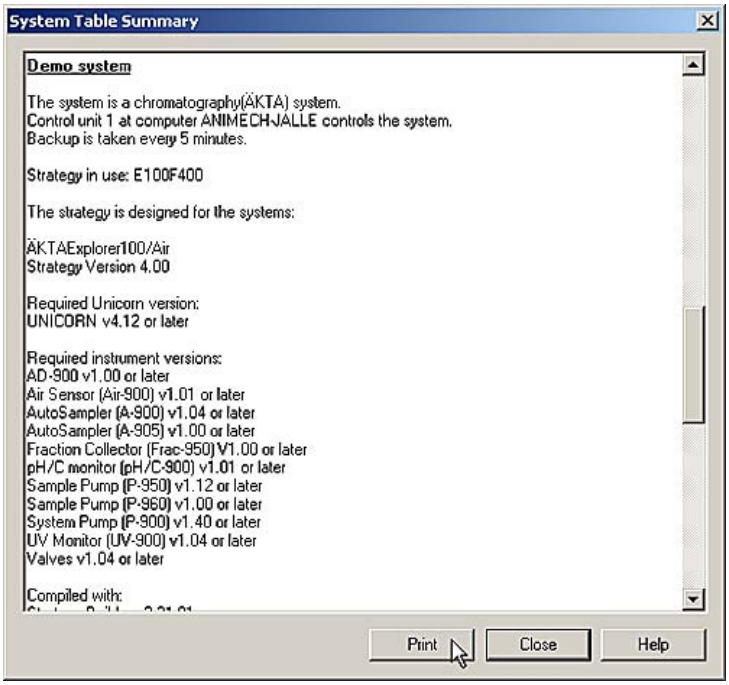
How to view or print a system summary

You can view and print a total summary of a selected system from the ***System Table Summary*** dialog box.

The table below describes how to view and print an information summary of a selected systemthe systems:

Step	Action
1	Choose ***Administration:System Setup*** in the ***UNICORN Manager***. *Result*: The ***System Setup*** dialog box is displayed:



Step	Action
2	• Select the system you want a summary of. • Click the ***Summary*** button. *Result*: The ***System Table Summary*** dialog box is displayed: 
3	• Click the ***Print*** button to print the information. • Click the ***Close*** button to exit the dialog box.

3.6 How to back up and restore system data

Introduction

You can create a backup file with system information and store it on a USB memory or another drive. The backup file will contain information about

- Global Files
- Personal Files
- System Files

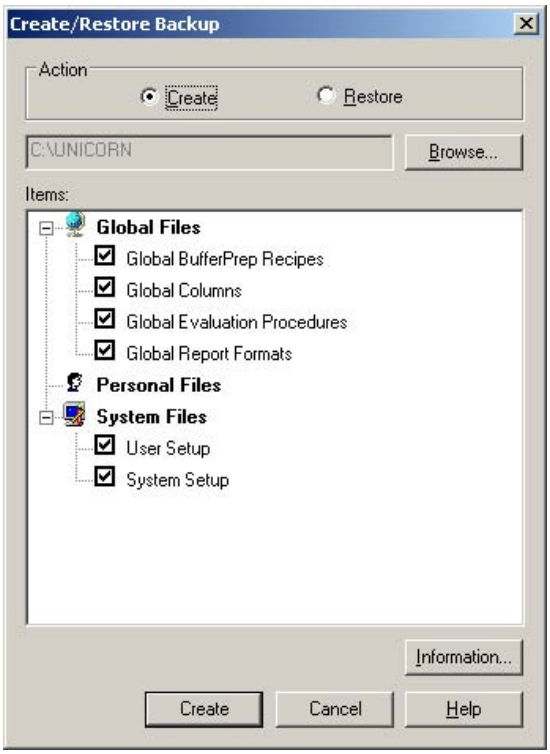
Afterwards you can use the backup file to restore the system definitions in case they are corrupted.

How to create a backup file

The table below describes how to create a backup file and store it for example on a USB memory:

Step	Action
1	Insert a USB memory into the computer if you want to store the backup file on a USB memory.

Step	Action
2	Choose ***Administration:Create/Restore Backup*** in the ***UNICORN Manager*** to display the ***Create/Restore Backup*** dialog box:

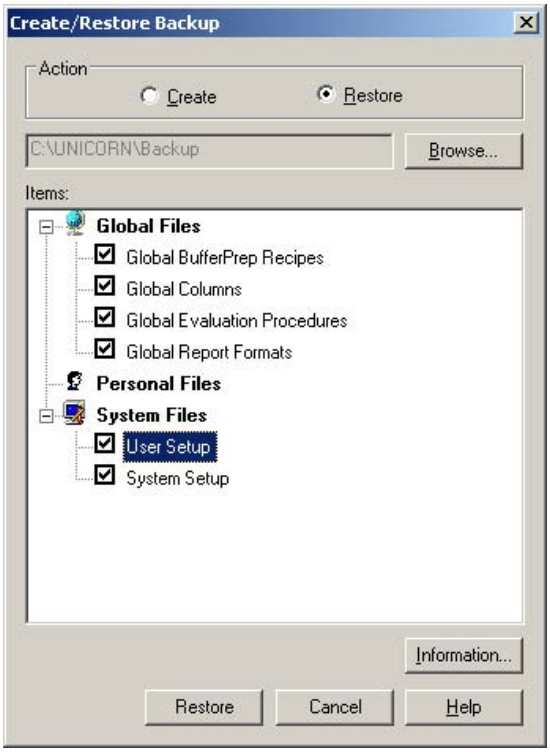


3	• In the ***Action*** field, make sure that the ***Create*** option is selected. • Click the ***Browse*** button to select where to store the backup file. • In the ***Items*** field, select which information to include on the backup file. • Click the ***Create*** button to create the backup file and store it in the selected location. **Note:** You can click the ***Information*** button to see which information files will be included in the backup file.

How to restore the system data

The table below describes how to restore the system data from a backup file, located for example on a USB memory:

Step	Action
1	If the backup file is located on a USB memory, insert this into the computer.
2	Choose ***Administration:Create/Restore Backup*** in the ***UNICORN Manager*** to display the ***Create/Restore Backup*** dialog box:



Step	Action
3	• In the ***Action*** field, select the ***Restore*** option. • Click the ***Browse*** button to select the folder where the backup file is located. • In the ***Items*** field, select which information to include from the backup file. • Click the ***Restore*** button to restore the system definitions. **Note:** You can click the ***Information*** button to see which information files are included in the backup file.

3.7 How to set up a printer

Introduction

UNICORN uses the default printer and printer settings that are installed on your computer. You can change your printer by changing the default Windows settings, but you can also set up a printer in UNICORN for the current working session.

How to set up a printer

The table below describes how to set up a printer in UNICORN.

Step	Action
1	Select the ***File:Printer Setup*** menu command in the ***UNICORN Manager*** module. *Result*: The ***Print Setup*** dialog box opens.
2	Select a printer from the ***Name*** drop-down box.
3	Change all printer ***Properties*** as necessary.
4	Change ***Paper*** and ***Orientation*** settings as necessary.
5	If you wish to access a network printer that is not shown in the ***Name*** drop-down box: • Click the ***Network...*** button *Result:* The ***Connect to Printer*** dialog box opens. • Locate and select the network printer by browsing the network in the ***Shared printers*** field. • Click ***OK*** to select the printer and close the ***Connect to Printer*** dialog box.
6	Click ***OK*** in the ***Print Setup*** dialog box to complete the setup.

Note: To save created reports electronically you can select to print the files in PDF-format. To be able to do this you must have a full version of Adobe™ Acrobat™ installed and select PDF Writer or Distiller™ in the ***Printer Setup***. Other compatible PDF software will serve the same purpose.

4 Files and folders in UNICORN

Introduction

All UNICORN data is organized in files and folders. Files and folders are handled like in any other Windows application, with some exceptions. This chapter describes how to work with UNICORN files and folders, with the focus on the topics that are specific for UNICORN.

In this chapter

This chapter contains these sections.

Section	See page
4.1 How to create folders	84
4.2 How to open and preview files	85
4.3 How to arrange and locate your files	88
4.4 How to copy, delete, rename and backup files and folders	92

4.1 How to create folders

Introduction

This section describes how folders are organized in UNICORN and how to create a new user-specific folder for the user's methods and results.

UNICORN folders

The files and folders are displayed in the two ***UNICORN Manager*** module windows.

- All method files and corresponding folders are listed in the ***Methods*** window.
- The result files and folders are listed in the ***Results*** window.
- You can only see folders that you have access to.
- You can only see method files that are written for systems that you have access to.

How to create a user-specific folder

The table below describes how to create a user-specific folder.

Step	Action
1	Select the window you want to create the folder in: ***Methods*** or ***Results***. (*Result*: The window title bar is highlighted.)
2	• Select ***File:New:Folder***. *or* • Right-click and select the ***New Folder*** shortcut. *Result*: The ***Create New Folder*** dialog box opens.
3	Type a name for the new folder.
4	Click ***OK***.

4.2 How to open and preview files

Introduction

This section describes how to open your saved method files and result files. You can also preview your result files to identify the correct file before you open it.

How to open a method file

You open a method file in the ***UNICORN Manager*** module. Click the file in the ***Methods*** window to select it and

- choose ***File:Open***.

or

- right-click the file and choose ***Open*** from the short-cut menu.

or

- double-click the file.

Result: The file is opened for editing in the ***Method Editor*** module.

Note: A method file cannot be opened on two workstations simultaneously.

How to open a result file in UNICORN Manager

You can open a result file in the ***UNICORN Manager*** module. Click the file in the ***Results*** window to select it and

- choose ***File:Open***.

  or

- right-click the file and choose ***Open*** from the short-cut menu.

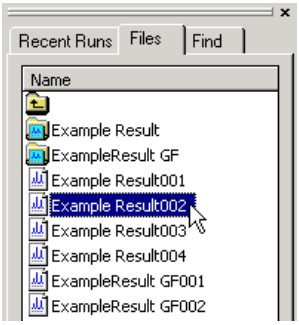
  or

- double-click the file.

Result: The file is opened for editing in the ***Evaluation*** module.

How to open a result file in the Evaluation module

The table below describes how to open a result file from the ***File Navigator*** in the ***Evaluation*** module.

Step	Action
1	• Click the ***Files*** tab.
2	• Locate and double-click the result file  *Result*: The result file opens.

Note: The ***File Navigator*** opens by default in the ***Evaluation*** module. If it has been closed, select ***View:File Navigator*** in the ***Evaluation*** module.
The ***File Navigator*** is described further in *Section 10.2 How to use the File Navigator, on page 269*.

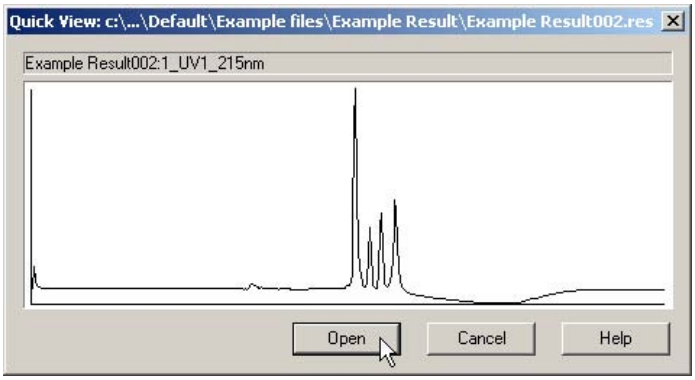
Quick View

Quick View is a preview function for result files to make it easier to select the correct result file.

You can preview the first curve in the first chromatogram. You can also select to view another curve as default by selecting another curve number in your ***User Attributes*** settings, see *Section 3.4 How to change your passwords and user attributes, on page 69*. Several files can be opened for comparison.

How to use Quick View

The table below describes how to preview result files in Quick View.

Step	Action
1	Select one or more result files in the ***Result*** window of the ***UNICORN Manager***.
2	• Choose ***File:Quick View***. *or* • Right-click and choose ***Quick View*** from the short-cut menu. *Result*: The ***Quick View*** dialog box opens. 
3	• Click the ***Next*** and ***Previous*** buttons to move between the result files (if more than one is selected). • Click the ***Open*** button when the right file is displayed. *Result*: The result file that is displayed in the dialog box opens in the ***Evaluation*** module.

4.3 How to arrange and locate your files

Introduction

This section describes how to arrange the way the files are displayed in your UNICORN workspace and how to locate files through a search.

Different view modes

You can choose how the files and folders are displayed in the ***UNICORN Manager*** windows. The options are the standard Windows alternatives:

- Details
- List
- Large icons
- Small icons.

How to change the view mode

If you want to change the view you either:

- Select ***View*** and the option that you want,

  or

- Right-click and select ***View*** and the option that you want from the shortcut menu.

Sort order in detailed view

The files can be sorted in a different order when a window is displayed in detailed view. The table below shows the options.

Sorted by:	Order
Name	Alphabetical order or reverse alphabetical order.
System	Alphabetical order or reverse alphabetical order (***Method*** window only).
Size	Smallest or largest files first.
Type	Alphabetical order of file extension type.
Modified	Most recently modified files first.

Sorted by:	Order
Created	Most recent creation dates first.

How to change the sorting order

Select one of the methods below to change the sorting order:

- Select ***View:Sort*** and the option that you want,

  or

- Right-click and select ***Sort*** and the option that you want from the short-cut menu.

  or

- Click the column header for the option that you want to sort by (a second click on the same header will reverse the order).

Note: Only the currently active window is affected.

How to filter Method files

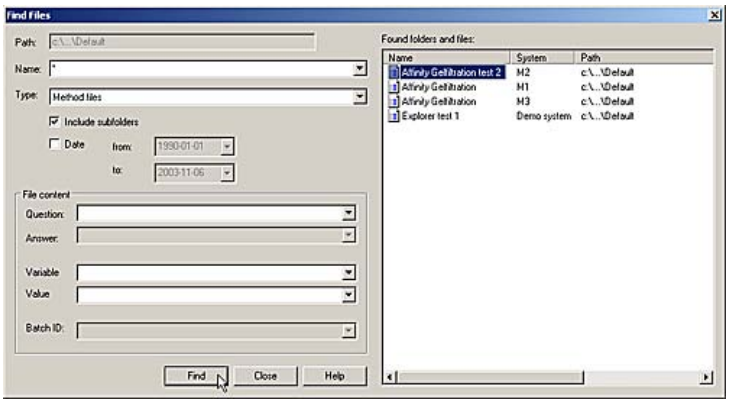
The files in the ***Method*** window can be filtered to show only methods for selected systems. You can also limit the displayed files by using standard Windows wildcard characters. The title bar of the ***Method*** window indicates if a filter has been activated.

The table below describes how to activate a filter.

Step	Action
1	• Select ***View:Filter***. *or* • Right-click and select ***Filter*** from the shortcut menu. *Result*: The ***Filter*** dialog box opens.
2	Click the check-boxes for the systems for which you want to show files.
3	Enter a file name specification (if necessary).
4	Click ***OK***.

How to find files

The table below describes how to perform a search for files.

Step	Action
1	Click either the ***Methods*** or ***Results*** window and: • Select the ***File:Find*** menu command. or • Right-click and select ***Find*** from the shortcut menu. *Result*: The ***Find files*** dialog box opens. 
2	Add search criteria to the dialog box, for example: • Type a name in the ***Name*** field. • Select a file type from the ***Type*** drop-down box. • Select if the search should include subfolders. • Select date limits in the ***Date*** drop-down boxes. • Type text strings to match ***Question*** or ***Answer*** texts. • Type a variable name and, if desired, a value. • Type a ***Batch ID***. **Note:** You can search for a sample ID provided the sample ID is defined as a variable.

Step	Action
3	Click ***Find***. *Result*: The search results are listed in the ***Found folders and files*** field. The search is limited to either methods or results and to the folder (including its subfolders) that is currently displayed.
4	Double-click a file in this list. *Result*: The dialog box is closed and the selected file is highlighted in the ***UNICORN Manager*** window. **Note:** If you click ***Close*** you will return to the ***UNICORN Manager*** window with no file highlighted regardless if you have selected one in the dialog box or not.

4.4 How to copy, delete, rename and backup files and folders

Introduction

UNICORN has some file and folder handling functions that are slightly different from the general Windows functions. This section focuses on the differences.

Note: You need explicit authorization in your user profile to copy, move and delete files.

How to copy or move files and folders

There are some restrictions to how you can copy or move files and folders:

- Files and folders can only be copied or moved to folders that are specific to your user name.
- You can also copy files to and from the folders that you have access to on the network.
- Method files or folders cannot be copied to the ***Results*** window.
- Result files and folders cannot be copied to the ***Methods*** window.

If you copy a folder you will also at the same time copy all files and folders that it contains. The table below describes how to copy files and folders.

Note: Follow the same steps but select ***Move*** to move files and folders.

Step	Action
1	Select one or more files and folders in either the ***Methods*** or ***Results*** window of the ***UNICORN Manager***.
2	• Select ***File:Copy***. *or* • Right-click and select ***Copy*** from the short-cut menu. *Result*: The ***Copy*** dialog box is opened.
3	Select a target folder or USB memory.
4	Click ***OK***.

The function Copy to External

Use the function ***Copy to External*** when you need to copy files and folders outside of your own user folders. ***Copy to External*** should be used specifically when you need:

- to copy a method to another system (the method can then be connected to the appropriate system),
- to copy to a USB memory.

How to Copy to External

The table below describes how to use the function ***Copy to External***.

Step	Action
1	Select the file you want to copy.
2	• Select ***File:Copy to External***. *or* • Right-click and select ***Copy to External*** from the shortcut menu. *Result*: The ***Copy to External*** dialog box opens.
3	Select the destination drive and folder.
4	Click the ***Save*** button.

The function Copy from External

The function ***Copy from External*** can be used to import files and folders:

- If the files were saved using the function ***Copy to External*** they will automatically be decompressed.
- Copied method files must be connected to the same type of system they originally were created for. This is part of the ***Copy from External*** procedure.
- Method files that have been copied in and connected are displayed in the designated folder in the ***Methods*** window.

How to use Copy from External

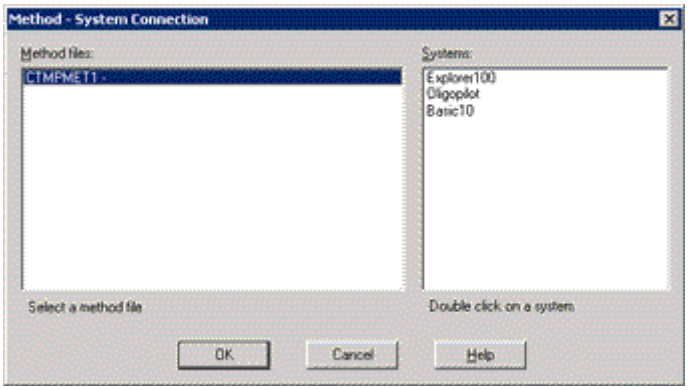
The table below describes how to use the function ***Copy from External***.

Step	Action
1	Select a destination folder in the ***Methods*** or the ***Results*** window.
2	• Select ***File:Copy from External***. *or* • Right-click and select ***Copy from External***. **Note:** Do not select a file icon. *Result*: The ***Copy from External*** dialog box opens.
3	Select the files you want to copy.
4	Click ***Save***. *Result*: • Result files are copied into the designated folder in the ***Results*** window. • If method files were selected, the ***Method-System Connection*** dialog box opens.

How to connect a method to a system

The table below describes how to connect a method to a system.

Step	Action
1	Select a method and double-click a system.



Result: The method is connected and the system name is added after the method name in the ***Method files*** list.

2	Repeat step 1 until all methods are connected to a system.
3	Click ***OK***.

How to rename files and folders

The table below describes how to rename files and folders in the ***Methods*** or ***Results*** windows in the ***UNICORN Manager*** module.

Step	Action
1	Select the item that you want to rename.
2	• Select ***File:Rename***. or • Right-click and select ***Rename*** from the shortcut menu. *Result*: The ***Rename*** dialog box opens.
3	Type a new name.

Step	Action
4	Click ***OK***.

How to delete files and folders

The table below describes how to delete files and folders in the ***Methods*** or ***Results*** windows in the ***UNICORN Manager*** module.

Note: Home folders cannot be deleted this way.

Step	Action
1	Select the item that you want to delete.
2	• Select ***File:Delete***. or • Right-click and select ***Delete*** from the shortcut menu. or • Press the ***Delete*** key.
3	Confirm the delete action in the confirmation dialog box

Backup security

Backup copies should be taken regularly to avoid data loss in the event of hard disk failure or accidental deletion. You can use the function ***Copy to External*** to save your files on the network server.

Note: GE Healthcare cannot accept responsibility for the replacement of method or result files that were lost as a result of computer failure or other incidents.

5 How to create a method

Introduction

Chromatography runs are programmed as ***Methods*** in UNICORN. Before you can proceed with a chromatography run you need either to use an existing method or create a new method. This chapter describes how to create new methods. It also contains instructions for signing a method.

In this chapter

This chapter contains these sections:

Section	See page
5.1 How to use the Method Wizard	98
5.2 How to use the Method templates	103
5.3 How to use Text instructions	106
5.4 How to sign the method	110

5.1 How to use the Method Wizard

Introduction

This section describes how to use a ***Method Wizard*** to create a new method. For most purposes customized methods can be created simply by setting appropriate values for the method variables.

Note: Each method is written for a specific strategy. The function of the method cannot be guaranteed on systems having other strategies.

Are wizards always available?

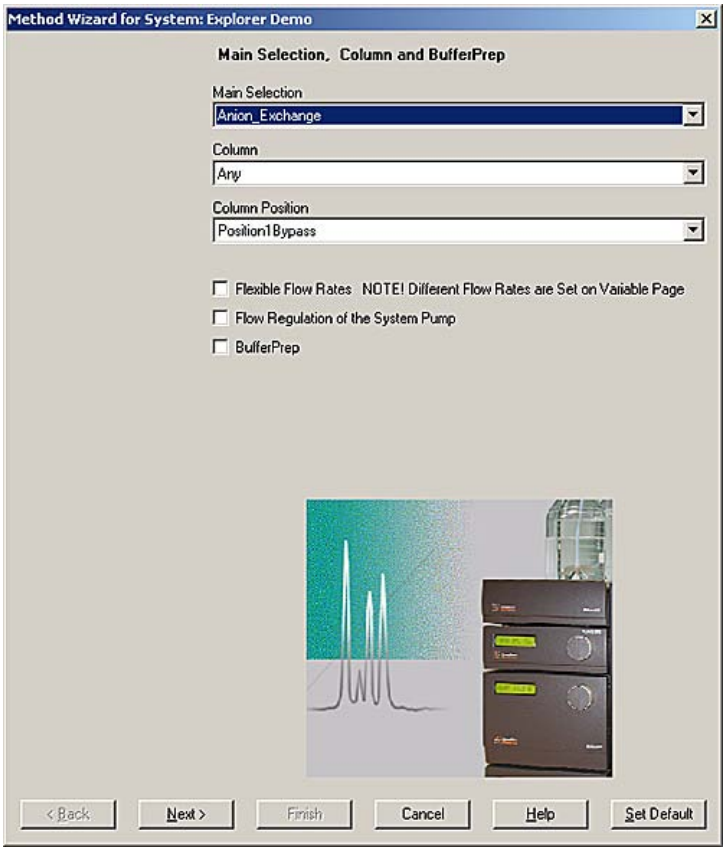
Method Wizards are available for some ***ÄKTAdesign*** systems delivered with standard strategies. ***Method Wizards*** are not available for process systems.

How to create a new method

The table below describes how to create a method with the ***Method Wizard***.

Step	Action
1	Click the ***Method Wizard*** icon on the ***Method Editor*** module or choose ***File:Method Wizard***.

Result: The ***Method Wizard*** dialog box appears.

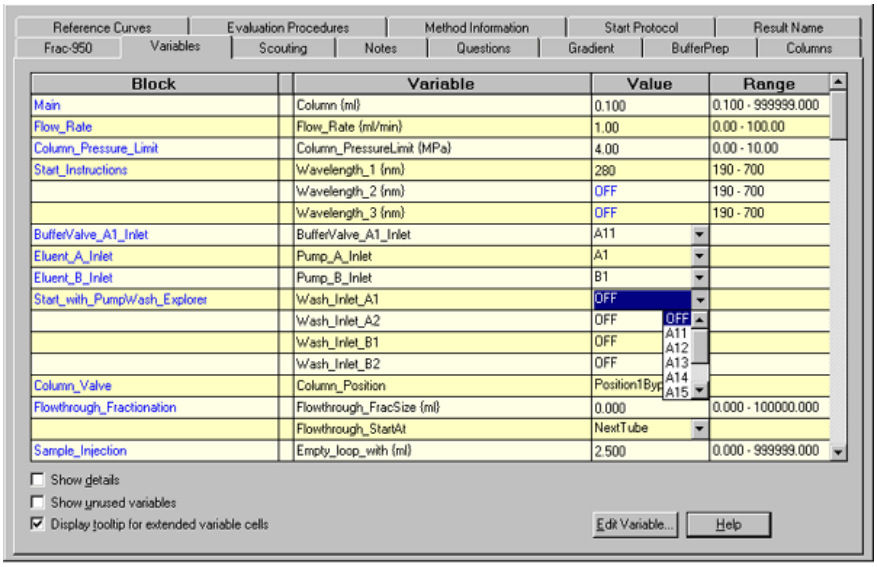


Note: If several systems are available you must first select which system you want to use.

Step	Action
2	Select the appropriate parameter values and click the ***Next*** button. *Note:* Click ***Set Default*** on the first wizard page to restore all settings to the default values.
3	In each new dialog box, select the appropriate parameter values and click the ***Next*** button to continue. *Note:* Select a column even if you want to perform a test run without a column. Use a small column. Replace the column with a piece of tubing when you run the method.
4	Click the ***Finish*** button in the last dialog box. *Result*: The ***Run Setup*** opens.

The Run Setup

The ***Run Setup*** consists of a number of tabs. Click on the appropriate tab at the top to select it.



The Variables tab

The method is represented by a number of blocks on the ***Variables*** tab. The blocks are typical steps in a chromatographic run.

Each block contains a number of ***Method Variables*** with suitable default values that can be changed to suit your application. Only the most commonly used variables are initially shown on the page. Click the ***Show details*** check box to display all variables in the method.

Default values for columns

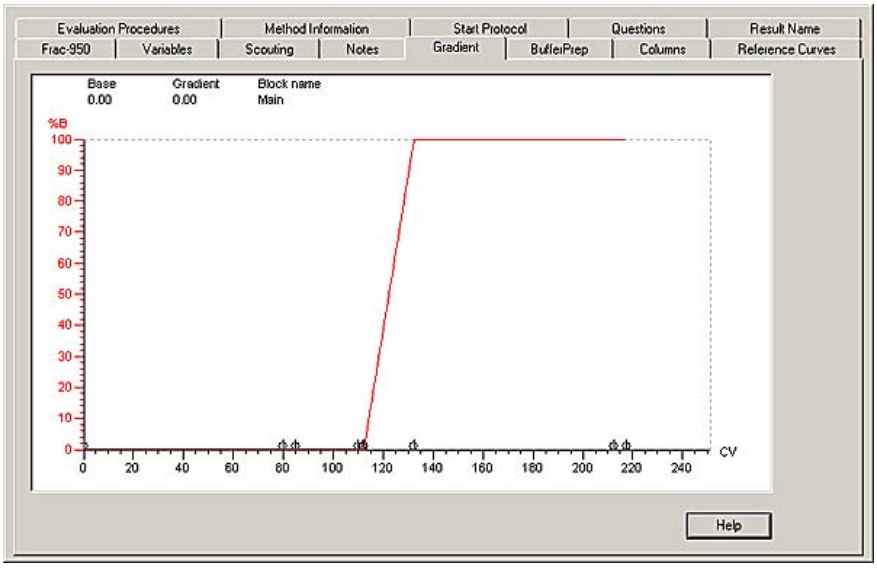
When you select a column, default values will be set for several parameters including the following:

- the correct column volume
- the recommended flow rate
- the correct pressure limit.

Note: If you exceed the recommended values for the selected column you will receive a warning when you save your method.

The Gradient tab

The ***Gradient*** tab shows the method graphically:



The length of each block is marked at the bottom of the graph.

- Click the X-axis to view the method in time, volume or column volumes.
- Drag the Y-axis to display a marker in the gradient. The ***Base*** value, ***Gradient*** value and ***Block name*** at the current marker position will be displayed in the upper part of the graph.

How to save the new method

A new method created from a ***Wizard*** is untitled, and must be saved under a method name before it can be used. The table below describes how to save a new method.

Step	Action
1	Click the ***Save Method*** toolbar or choose ***File:Save***.
2	• If required, save the method in a folder other than the default home folder. • Enter a ***Method name*** for the method. The total path can be up to 256 characters long. The method name must be unique for the chosen system within the folder.
3	• If you have more than one system connected to the computer, choose the ***System*** for which the method is intended. The method can be run on any system that uses the same strategy. Remember that different systems may have different configurations and control capabilities. • Choose the ***Technique*** for which the method was written.
4	Click ***OK***. *Result:* The method is saved, but remains open in the ***Method Editor***, so that you can continue editing if you wish.

Note: You might want to sign your method. If you do so, you can choose to lock the method so that nobody will be able to change the method. See *Section 5.4 How to sign the method, on page 110* for further instructions.

5.2 How to use the Method templates

Introduction

This section describes how to create methods based on an existing template.

Note: A custom system, for example a process system, requires that the users create their own templates by saving methods as templates. Each method is written for a specific strategy. The function of the method cannot be guaranteed on systems having other strategies.

How to create a new method

The table below describes how to create a method from the ***UNICORN Manager*** module.

Note: The ***New Method*** dialog box is also accessible from the ***Method Editor*** module using the same commands.

Step	Action
1	• Choose the ***File:New:Method*** menu command *or* • click the ***New Method*** icon. *or* • right-click in the ***Methods*** window and select ***New:Method*** from the shortcut menu. *Result*: The ***New Method*** dialog box opens in the ***Method Editor*** module.

Step	Action
2	• Select the system for which you want to create the method in the ***For system*** drop-down list. • Select ***Template*** in the ***Use*** field. • Select a chromatographic technique from the ***Technique*** drop-down list. • Select a method template from the ***Template*** list. • Select a column from the ***For column*** list and click ***OK***. *Result:* The method template will be opened as an untitled method in the ***Run Setup*** in the ***Method Editor***. *Note*: If ***Any*** is selected in the ***For column*** list, you can use any column but must enter the column volume in the method on the ***Variables*** tab. It is recommended that a specific column is selected.

Note: Only columns for the selected technique are displayed. If Any is selected as technique, all columns are displayed. Right-click in the textbox to open a list of the column categories to limit the number of displayed columns. If you type the beginning of a column name in the textbox UNICORN will automatically complete the column name.

If you do not find your specific column it can be added to the list. The column value, recommended flow rate, pressure limit and averaging time for the selected column will be automatically copied into the method, thus reducing the need to edit the method.

Method notes

Click the ***Notes*** and then the ***Method Notes*** tabs in the ***Run Setup***. The notes describe important information about the template and how the system should be connected so that the method will work correctly.

Note: If your system does not correspond to the description on the ***Method Notes*** tab, either:

- rearrange the valves and tubing connections in accordance with the method notes description

or

- edit the method instructions in accordance with your system setup.

How to save the new method

A new method created from a method template is untitled, and must be saved under a method name before it can be used.

The table below describes how to save a new method.

Step	Action
1	Click the ***Save Method*** toolbar icon or choose ***File:Save***.
2	• If required, save the method in a folder other than the default home folder. • Enter a ***Method name*** for the method. The total path can be up to 256 characters long. The method name must be unique for the chosen system within the folder.
3	• If you have more than one system connected to the computer, choose the ***System*** for which the method is intended. The method can be run on any system that uses the same strategy. Remember that different systems may have different configurations and control capabilities. • Choose the ***Technique*** for which the method was written. • Click ***OK***. *Result:* The method is saved, but remains open in the ***Method Editor***, so that you can continue editing if you wish.

Note: You might want to sign your method. If you do so, you can choose to lock the method so that nobody else will be able to change the method. See *Section 5.4 How to sign the method, on page 110* for further instructions.

5.3 How to use Text instructions

Introduction

You can use the ***Text Instructions*** editor in the ***Method Editor*** to build your method step by step. You can also use the editor to modify instructions in methods created by wizards or based on templates.

Advanced editing facilities are available when you work directly in the ***Text Instructions*** editor. This section is a very brief description of this process. See *Chapter 6 How to edit methods, on page 111* for detailed instructions.

Note: Each method is written for a specific strategy. The function of the method cannot be guaranteed on systems having other strategies.

When do I use Text Instructions?

Use ***Text Instructions*** when you want:

- to change selected instructions in the method, for example the outlet valve position
- to add blocks or instructions, for example ***Watch*** instructions
- to change method instructions to adapt to non-standard system configurations
- to create new methods for applications not covered by the supplied templates or wizards.

How to edit Text Instructions

Open the ***Text Instructions*** editor by following the steps in the table below.

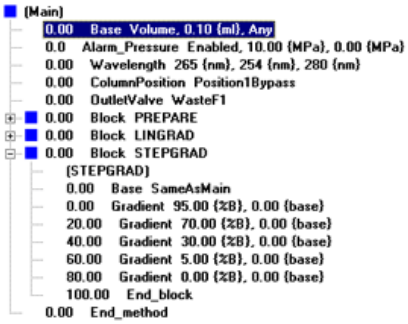
Step	Action
1	Select the ***Method Editor*** module and click the ***Text Instructions*** icon.

Step	Action
2	• Click the ***Customise Panes*** icon and select ***Text*** and ***Instruction Box***. • Click ***OK***.
3	Select instructions in the ***Instruction box*** in the lower part of the ***Method Editor***, and use the ***Insert***, ***Change***, ***Replace*** or ***Delete*** buttons. All text entries are shown in the ***Text*** pane. Applicable variables can be edited for each selection. The illustration below shows the ***Instruction box***:

Instructions can be organized in blocks

Individual text instructions can be grouped in blocks of instructions (marked by blue square symbols) for a specific functional use, e.g. to load a sample, to equilibrate a column etc. A block may contain other blocks or individual instructions.

This is an example of text instructions in the ***Text*** pane:


(Main)
0.00 Base Volume, 0.10 (ml), Any
0.0 Alarm_Pressure Enabled, 10.00 (MPa), 0.00 (MPa)
0.00 Wavelength 265 (nm), 254 (nm), 280 (nm)
0.00 ColumnPosition Position1Bypass
0.00 OutletValve WasteF1
0.00 Block PREPARE
0.00 Block LINGRAD
0.00 Block STEPGRAD
(STEPGRAD)
0.00 Base SameAsMain
0.00 Gradient 95.00 (%B), 0.00 (base)
20.00 Gradient 70.00 (%B), 0.00 (base)
40.00 Gradient 30.00 (%B), 0.00 (base)
60.00 Gradient 5.00 (%B), 0.00 (base)
80.00 Gradient 0.00 (%B), 0.00 (base)
100.00 End_block
0.00 End_method

How to save the new method

A new method is untitled, and must be saved under a method name before it can be used.

The table below describes how to save a new method.

Step	Action
1	Click the ***Save Method*** toolbar or choose ***File:Save***.
2	• If required, save the method in a folder other than the default home folder. • Enter a ***Method name*** for the method. The total path can be up to 256 characters long. The method name must be unique for the chosen system within the folder.
3	• If you have more than one system connected to the computer, choose the ***System*** for which the method is intended. The method can be run on any system that uses the same strategy. Remember that different systems may have different configurations and control capabilities. • Choose the ***Technique*** for which the method was written. • Click ***OK***. *Result:* The method is saved, but remains open in the ***Method Editor***, so that you can continue editing if you wish.

Note: You might want to sign your method. If you do so, you can choose to lock the method so that nobody will be able to change the method. See *Section 5.4 How to sign the method, on page 110* for further instructions.

How to display descriptions of instructions

A dedicated strategy is available for each system in the ***ÄKTAdesign*** platform. Although the majority of the instructions are general, some of them differ slightly between the individual strategies.

The list below describes two ways to display descriptions of the instructions in your particular strategy:

- Select the instruction in the ***Instruction Box*** of the ***Method Editor*** and press ***<F1>***

or

- Right-click the instruction in the ***Text*** pane and choose the menu option ***What's This?***

How to print descriptions of instructions

The table below describes how to print descriptions of the instructions in your particular strategy:

Step	Action
1	Select ***File:Print*** in the ***Method Editor***.
2	• Select the ***Instruction set*** option to print the full set of instructions. • Click ***OK***.

How to add a Snapshot

The ***Snapshot*** instruction can be used to record the curve values at a specific point in the method run. For example, a snapshot can be inserted to record the curve values immediately before an injection. The values are recorded in the result file and can be viewed in the ***Snapshots*** tab of the ***Documentation*** dialog box (See *Section 10.7 Run documentation, on page 327*). Up to 500 snapshots can be recorded in each result file. The table below describes how to add a snapshot instruction to a method:

Step	Action
1	• In the ***Text*** pane, select the instruction immediately before the position where you want to insert the ***Snapshot*** instruction.
2	• Select ***Other*** in the ***Instructions*** field of the ***Instructions box***. • Select ***Snapshot*** in the instructions list.
3	Type a name in the ***Name*** text box in the ***Parameters*** field. • Click the ***Insert*** button.

Note: Snapshots can also be taken in the ***System Control*** and ***Evaluation*** modules. However, these snapshots will only record the data for a specific moment. For more information about the ***Snapshot*** function see *Section 2.2.7 Snapshots, on page 50*.

5.4 How to sign the method

Instruction

If you sign the method, you can choose to lock it so that nobody will be able to change it.

The table below describes how to sign the method.

Step	Action
1	Choose ***File:Sign Method*** in the ***Method Editor***. *Result:* The ***Sign the Method*** dialog box is displayed.
2	Click the ***Signing*** tab and do the following: • Select a user in the ***User*** drop-down list box. In most instances, you will want to use the current user shown on the list. • In the ***Meaning*** field, provide a short text description explaining the meaning behind the signature (for example "Method now fully tested and approved"). • Type your signature password in the ***Password*** field. If desired, select the ***Lock*** box to lock the method permanently from further changes by other users. • If needed, view a list of all signatures associated with the current method on the ***View Signatures*** tab. • Click ***OK*** on either the ***Signing*** or ***View Signatures*** tab.

6 How to edit methods

Introduction

This chapter describes the complete facilities for editing methods in UNICORN. For many applications, suitable methods can be created by changing the default values in one of the wizard-generated methods supplied with UNICORN.

Use the more advanced editing facilities described here when you want

- to change selected instructions in the method, for example, change the outlet valve position
- to add blocks and instructions
- to change method instructions to adapt to non-standard system configurations.

In this chapter

This chapter contains these sections:

Section	See page
6.1 The Method Editor interface	112
6.2 Method blocks	118
6.3 Method instructions	134
6.4 How to use method variables	145
6.5 Run Setup	149
6.6 How to use selected method instructions	188
6.7 Standard Watch conditions	202
6.8 How to save or delete a method template	208
6.9 How to print a method	210
6.10 How to export a method	212

6.1 The Method Editor interface

Introduction

This section contains a general description of the ***Method Editor*** user interface and the editing operations that can be performed in the different parts of the module.

In this section

This section contains these topics:

Section	See page
6.1.1 Method Editor module	113
6.1.2 Text Instructions editor	115

6.1.1 Method Editor module

Two modes

The ***Method Editor*** interface operates in two modes:

- ***Text Instructions*** editor for entering and editing method instructions (see *Section 6.1.2 Text Instructions editor, on page 115*)
- ***Run Setup*** for defining method properties (see *Section 6.5 Run Setup, on page 149*).

How to open the Method Editor dialog boxes

The table below describes how to open the dialog boxes in the ***Method Editor***:

If you want to open...	then...
the ***Text Instructions*** editor	click the ***Text Instructions*** icon. *or* choose ***View:Text Instructions***.
the ***Run Setup***	click the ***Run Setup*** icon. *or* choose ***View:Run Setup***.
the ***Log Format***	click the ***Log Format*** icon. *or* choose ***View:Log Format***.

If you want to open...	then...
the ***Method Wizard***	click the ***Method Wizard*** icon. *or* choose ***File:Method Wizard***.

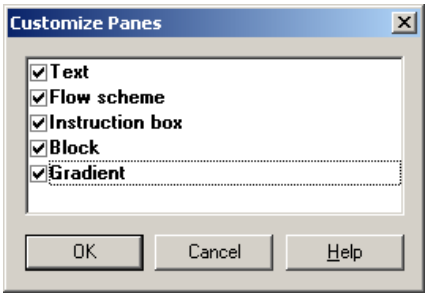
6.1.2 Text Instructions editor

How to select panes to be displayed

You have a choice of four panes that can be open together with the ***Instruction box*** in the ***Text Instructions*** editor, all at once or one at a time.

Follow the steps in this table to select the panes to be displayed:

Step	Action
1	• In the ***Method Editor***, choose ***View:Text Instructions*** *or* • click the ***Text Instructions*** icon.
2	• Choose ***View:Panes:Customize*** (or select additional panes here) *or* • click the ***Customize Panes*** icon.

Step	Action
3	**Select panes** • Select panes in the dialog box and click the ***OK*** button.  **Deselect panes** • Deselect panes in the ***Customize Panes*** dialog box and click the ***OK*** button. *or* • right-click a window and select ***Hide***.

Method editing operations performed in the different panes

This table shows the method editing operations that can be performed in the different panes:

The pane...	Is used...	See section
Text	• to display instructions • to display and hide block instructions. • to select current instruction. • to edit instructions • to cut, copy and paste instructions. • to move instructions within a breakpoint.	*Section 6.2.1 How to view method blocks, on page 119* *Section 6.3 Method instructions, on page 134*

The pane...	Is used...	See section
Flow scheme	• for information only. This window is not updated according to system status and changes in the method.	*Section 9.2.4 The Flow Scheme pane, on page 247*
Instruction box	• to specify breakpoints, instructions, parameters and variables. • to insert, change and delete instructions.	*Section 6.3.2 How to add method instructions, on page 137*
Block	to select or display blocks.	*Section 6.2 Method blocks, on page 118*
Gradient	to display block duration and eluent gradient throughout the method.	*Section 6.5.5 The Gradient tab, on page 161*

6.2 Method blocks

Introduction

This section contains a description of how to organize a method in blocks of instructions in order to make it more structured, and of how to work with method blocks.

In this section

This section contains these topics:

Section	See page
6.2.1 How to view method blocks	119
6.2.2 How to call method blocks	121
6.2.3 How to add method blocks	122
6.2.4 How to delete method blocks	126
6.2.5 How to rename method blocks	129
6.2.6 How to find, copy and move method blocks	130
6.2.7 How to import method blocks	132

6.2.1 How to view method blocks

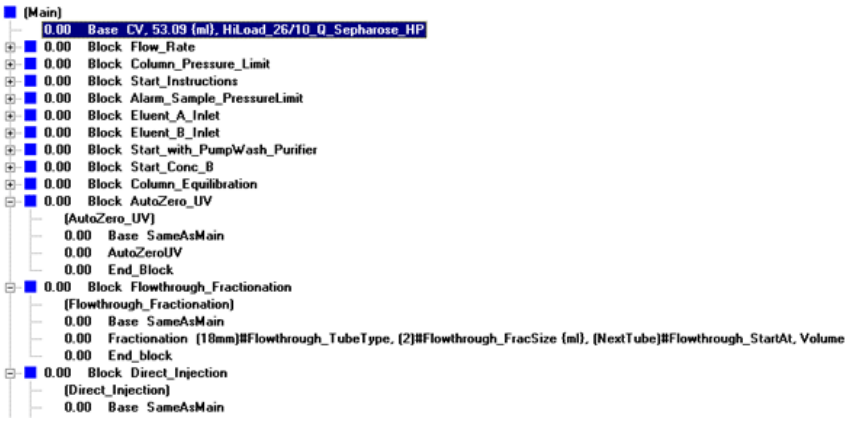
Instructions can be grouped into blocks

To view a method as a long list of individual text instructions can be confusing and inconvenient. Text instructions can therefore be grouped into blocks of instructions that define a specific functional use. For example, one block might contain the instructions necessary to equilibrate a column, and another block contains instructions to load a sample, etc.

The Text pane

In the ***Text*** pane of the ***Method Editor***, the method is shown as a list of blocks, denoted by the blue square symbols. Note that a block can also contain sub-blocks.

The figure below shows the text instructions in blocks:



The table below describes how to view or hide the instructions:

If you want...	then...
to view the instructions	click the "+" symbol *or* double-click the block name.
to hide the instructions	click the "-" symbol *or* double-click the block name.

The Block pane

The organization of blocks in the method is shown graphically in the ***Block*** pane of the ***Method Editor***.

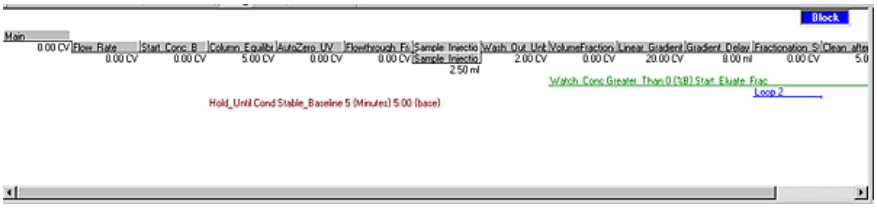
Description

Each block is represented by a gray bar with the block name and the length of the block. The line is shifted down to indicate calls to other blocks.

Click on the line that represents a block in the ***Block*** window to expand the block in the ***Text*** pane and select the first instruction in the block.

Figure

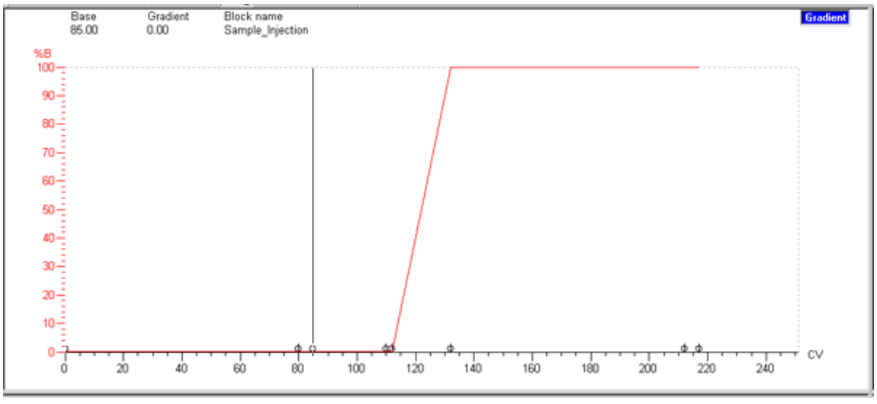
The figure below is an example with a ***Watch*** instruction to start the fraction collector which is active throughout the gradient elution block. ***Loop*** (to repeat a group of instructions) and ***Hold_until*** instructions are also indicated in the ***Block pane***.



The Gradient pane

Blocks are represented in the ***Gradient*** pane of the ***Method Editor*** by marks on the X-axis. The marks show the length of each block. The name of the block in which the cursor line is currently placed is shown at the top of the pane.

The figure below describes the ***Gradient*** pane:



6.2.2 How to call method blocks

General description

To execute the instructions contained within a block in a method, the block must be called by the program. When a block is called, the instructions in the block are executed in the order that they are written until the block is finished or the ***End_Block*** instruction is executed. Any settings made in a block are valid throughout the method until the settings are changed.

Types of calls

There are two types of calls:

- Unconditional calls, which are made with a ***Block*** instruction.
- Conditional calls, which are made with a ***Watch*** instruction. This makes it possible to call a specified block or an instruction when a particular monitor signal meets a given condition. As long as the condition is not met, the block is not activated.

Watch instructions

Watch instructions are indicated by a green line that show the start and duration of the watch. These instructions can use various conditions to respond to absolute signal values or to rate of signal changes.

The breakpoint when the ***Watch*** instruction is issued determines when the watch begins, not when the block is activated. Once set, a watch remains active until the condition is met or a new ***Watch*** instruction is issued for the same monitor. The watch is cancelled automatically when the condition is met. A watch can also be turned off with the ***Watch_off*** instruction.

See *Appendix F Method examples, on page 648* for more details on ***Watch*** instructions.

6.2.3 How to add method blocks

Two ways to add method blocks

You can add method blocks to a method in two ways, using either

- the ***Instruction box*** of the ***Text Instructions*** editor,

or

- the ***New Block*** dialog box reached via the ***New Block*** icon.

Both these alternatives are described below.

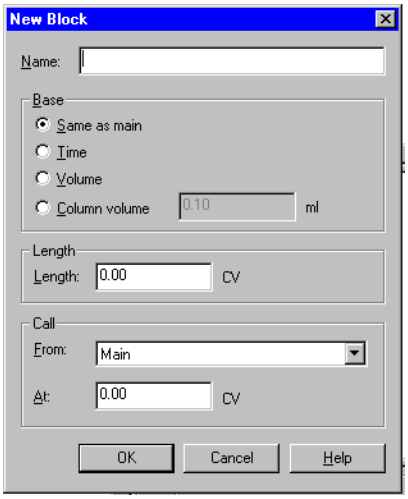
How to add blocks with the Instruction box

The table below describes how to add blocks with the ***Instruction box***:

Step	Action
1	In the ***Text pane*** of the ***Text Instructions*** editor, select the instruction or block that you want to precede the new block.
2	Select ***Other:Block*** in the ***Instruction box***.
3	• Enter a name for the block in the ***Block*** field. • Click the ***Insert*** button. *Result:* The block is inserted after the block that was selected in step 1.

The New Block dialog box

The illustration below shows the ***New Block*** dialog box that can be used when adding new method blocks:



How to add blocks with the New Block dialog box

The table below describes how to add blocks with the menu options of the ***New Block*** dialog box:

Step	Action
1	Choose ***Block:New*** in the ***Method Editor*** *or* click the ***New Block*** icon. *Result:* The ***New Block*** dialog box is displayed.

Step	Action
2	Enter the relevant information in the ***New Block*** dialog box, and click ***OK***. *Result:* The new block is added to the method, and placed last of all blocks. *Note*: The block can be placed in other positions by selecting something other than ***Main*** in the ***From*** droplist.

The fields of the New Block dialog box

The table below describes the fields of the ***New Block*** dialog box:

Field	Description
Name	Block names can be up to 30 characters long, and can contain letters (A-Z), digits (0-9) and the underscore character. Block names must be unique within the method. The case of letters is retained but not significant (the names ***Start_Frac*** and ***START_FRAC*** are treated as identical).
Base	One of the following options can be selected: • ***SameAsMain***: the new block will inherit the base from the ***Main*** block in the method. The corresponding ***Base*** instruction will be inserted in the block at breakpoint 0. • ***Time***: The block will be based on time. • ***Volume***: The block will be based on volume. • ***Column volume***: The block will be based on column volume.
Length	A block continues until the breakpoint for the ***End_Block*** instruction has been reached. An ***End_Block*** instruction will automatically be inserted in the block at the defined breakpoint. This field must not be left blank.

Field	Description
Call	You can call the new block from an existing block (for example the ***Main*** block). Select values in the two fields: • ***From*** The block from which the newly created block should be called. • ***At*** The breakpoint at which the call is to be made. If you do not want to call the block (for example when the block being created is to be activated by a ***Watch*** instruction), choose the ***<Unused>*** line from the ***From*** drop-down list. Blocks using this line are placed last in the method in the ***Unused*** category. *Note*: You should not call a block from within itself. If you do, you will generate a potentially infinite loop that exceeds the maximum number of calls allowed in a method. A loop symbol is displayed at the beginning of the line if this occurs.

6.2.4 How to delete method blocks

Four ways to delete blocks

There are four ways to delete blocks:

There are four ways to remove blocks from a method:

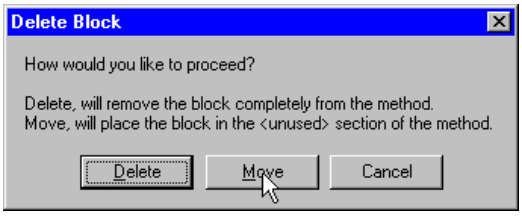
- To right-click a block and choose ***Delete*** from the shortcut menu
- To select a block and click ***Delete*** in the ***Instruction box***
- To select a block and press the <Delete> key on the keyboard
- To select a block and use the ***Block:Delete Block*** command

Note: When you use any of the first three ways, the ***Method Editor*** dialog box will give you the option to transfer the block to the Unused section.

Note: When you use the first three ways the block is only moved to the Unused section.

Delete options

The ***Delete Block*** dialog box is displayed when you delete a block with one of the first three options mentioned above.


Delete Block
How would you like to proceed?
Delete, will remove the block completely from the method.
Move, will place the block in the <unused> section of the method.
Delete
Move
Cancel

Options

Choose from the following options:

- ***Delete***: The block is totally removed from the method. If the block is called several times in the method, all the blocks will be deleted. Blocks deleted in this fashion cannot be called again in the method.

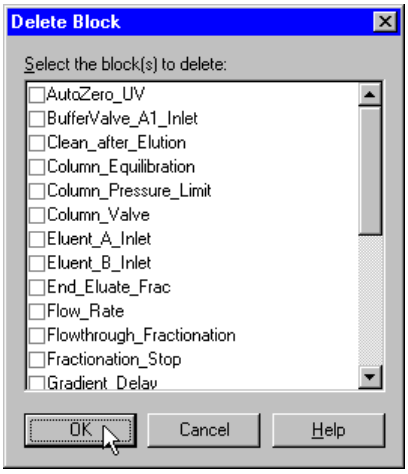
  Note: If the block contains sub-blocks, another dialog box is displayed, asking you if you want to delete the sub-blocks as well.

- ***Move***: The block is deleted from the method and transferred to the Unused section. If the block is called several times in the method, however, only the row with the block currently marked in the ***Text*** pane will be deleted. In this case, the block will not be placed in the Unused section (since the block is still used in the method). Blocks deleted in this fashion can be called again in the method.

How to use the Block:Delete Block command

The table below describes how to delete a block using the ***Block:Delete Block*** command:

Step	Action
1	Select the menu command ***Block:Delete Block*** in the ***Method Editor***. *Result:* The ***Delete Block*** dialog box is displayed with all blocks listed in alphabetical order.
2	Select the blocks you want to delete and click ***OK***.
3	Click ***Yes*** to confirm.



How to delete unused blocks

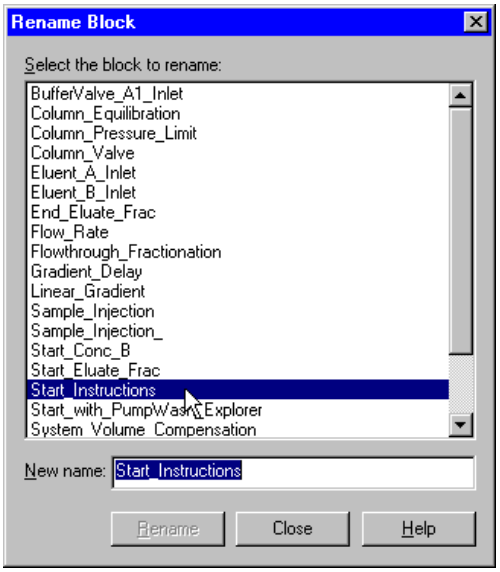
The table below describes how to delete an unused method block.

Step	Action
1	Highlight the method block. • Press the <delete> key *or* • Right-click and choose ***Delete*** on the shortcut menu. *Result*: The ***Delete Block*** dialog box opens. Note that the ***Move*** button is not available.
2	Click the ***Delete*** button. *Result*: The unused block is deleted and cannot be called upon again in the method.

6.2.5 How to rename method blocks

Instruction

The table below describes how to rename blocks:

Step	Action
1	Right-click the block you want to rename in the Text pane and select ***Rename***. *Result:* The ***Rename Block*** dialog box is displayed.  *Note:* By default, the block that is currently selected in the ***Text*** window is automatically selected in the dialog box.
2	Enter the new name in the ***New name*** field and click ***Rename***.
3	• If needed, repeat step 3 for other blocks. • Click ***Close***. *Note:* If the block you renamed is called in a ***Block*** or ***Watch*** instruction, the block name in these instructions will be changed automatically.

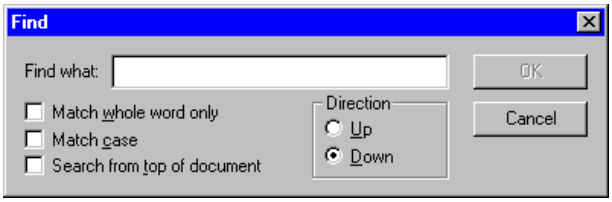
6.2.6 How to find, copy and move method blocks

Introduction

By using the ***Edit*** options in the ***Method Editor***, you can find, copy and paste and move blocks within a method.

How to find text strings in the method text

The table describes how to find text strings in the method text.

Step	Action
1	Choose ***Edit:Find*** in the ***Method Editor***, *or* right-click an instruction or a block in the ***Text*** window and select ***Find***. *Result:* The ***Find*** dialog box is displayed. 
2	• Enter the text you want to search for, search direction and case matching criteria. • Click ***OK***.

How to copy and paste a block

The table describes how to copy a block.

Step	Action
1	• Right-click the block you want to copy. • Choose ***Copy***.

Step	Action
2	• Right-click the instruction line just above the point where you want the block to be pasted. • Choose ***Paste***. *Result:* A dialog box asks if you wish to rename the pasted block.
3	Click ***Yes*** to rename the block before insertion, or ***No*** to insert the copied block directly. *Result:* The pasted block is inserted with the same breakpoint value as the block or instruction selected for point of insertion.

How to move a block

The table describes how to move a block.

Step	Action
1	• Right-click the block you want to move. • Choose ***Cut***.
2	• Right-click the instruction line just above the point where you want the block to be pasted. • Choose ***Paste***. *Result:* The block is now removed from its original breakpoint and pasted at the new breakpoint. The pasted block is inserted with the same breakpoint value as the block or instruction selected for point of insertion.

6.2.7 How to import method blocks

Introduction

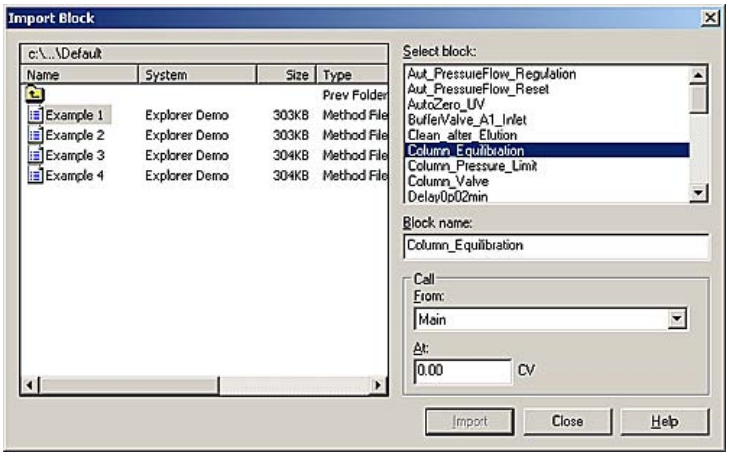
You can import method blocks from other method files. You can also use this function to copy blocks within a method. In the latter case, it is important to note that it is the *saved* version of the method that will be copied, not changes that have been made after you last saved the method.

The block is imported exactly as it appears in the source method. If the base of the imported block is defined as ***SameAsMain***, the block will inherit the main base in the new method, regardless of the base in the source method. Also, the imported block is inserted with the same breakpoint value as the block selected for point of insertion.

Instruction

The table below describes how to import method blocks:

Step	Action
1	Choose ***Block:Import Block As*** in the ***Method Editor***. *Result:* The ***Import Block*** dialog box is displayed.



2	• Select the method from which you want to import a block. • Select the block. *Result:* The name of the selected block is displayed in the ***Block name*** field.

Step	Action
3	In the ***Call*** field, do the following: • On the ***From*** drop-down list, select a block into which the block will be imported. • In the ***At*** field, select the breakpoint value for the block to be imported. Click the ***Import*** button. *Note:* The imported block cannot have the same name as an existing block in the method. If the default name is not allowed for this reason, the ***Import*** button will be gray and locked. If this occurs, change the name of the imported block so that the ***Import*** button becomes available.
4	• Repeat steps 2 and 3 if needed. • Click the ***Close*** button.

6.3 Method instructions

Introduction

This section describes how to work with the individual method instructions, in order to edit method blocks and methods.

In this section

This section contains these topics:

Section	See page
6.3.1 How to read method instructions	135
6.3.2 How to add method instructions	137
6.3.3 How to delete method instructions	139
6.3.4 How to change or move method instructions	140

6.3.1 How to read method instructions

Description of instruction markings

Method instructions are displayed in the ***Text*** pane of the ***Text Instructions Editor***. The table below explains the meaning of the markings:

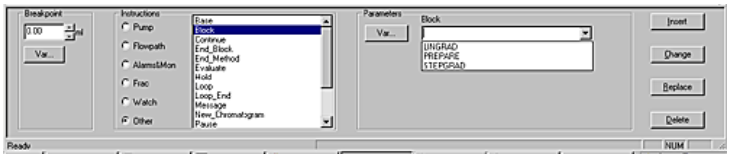
Marking	Explanation
Blue square beside text	Valid call instructions, that is, ***Block*** and ***Watch*** instructions to other blocks in the method.
Blue square with a red cross	Call instruction that contains one or more invalid instructions.
Bold text	Valid instructions.
Red dot	Instructions with invalid syntax. All such instructions must be deleted or changed before a method can be run. See *Section 6.3.4 How to change or move method instructions, on page 140*. The instructions may be of the following types: • Calls to blocks which are not defined in the method • Instructions that apply to a different system strategy (can occur if a method is written for one system and saved for another) • Instructions for components that have not been selected in the ***System Setup***.
Normal text	Instructions that will not be executed because • they are positioned after the end of a block or method *or* • they constitute a block to which there is no call.

Marking	Explanation
Text with a loop symbol	When a block is called from within itself this will generate a potentially infinite loop, which might exceed the maximum number of calls allowed in a method.

6.3.2 How to add method instructions

Instruction

The table below describes how to add a method instruction in the ***Text Instructions Editor***:

Step	Action
1	Select a block in the ***Text*** pane, and display the instructions within the block.
2	Select an instruction line in the block. Make sure that the selected instruction line is in the block, not the call to the block.
3	Open the ***Instruction box*** if it is not already displayed (***View: Panes***). Do the following: • Set the desired breakpoint in the ***Breakpoint*** field. • Choose the instruction type and the instruction in the ***Instructions*** field. For basic help on each instruction, click the instruction and press <F1>. • Type values for instruction parameters in the ***Parameters*** fields. If a scroll bar appears at the right side of the ***Parameters*** field, additional parameters are required. 
4	Click the ***Insert*** button. *Result:* The instruction will be inserted in the block • at the position of the breakpoint of the new instruction, if there are no other instructions at that breakpoint • immediately after the currently highlighted instruction, if the highlight is at the same breakpoint as the new instruction • as the last instruction at the breakpoint, if there are several instructions at the same breakpoint and none of these is highlighted. *Note:* Instructions that are placed at the same breakpoint are executed simultaneously, with the exception of ***Block*** instructions which are executed in the sequence in which they are written.

Pause, Hold and Hold_until instructions

If you use ÄKTA systems, the ***Pause***, ***Hold***, and ***Hold_until*** instructions will stop execution at this breakpoint, that is, instructions following after ***Pause***, ***Hold*** and ***Hold_until*** at the same breakpoint will not be executed until a ***Continue*** instruction is issued.

6.3.3 How to delete method instructions

Instruction

The table below describes how to delete method instructions in the ***Text Instructions Editor***:

Step	Action
1	Select the instruction in the ***Text*** pane.
2	Use one of the following alternatives: • Right-click the instruction and choose ***Delete*** in the displayed menu, *or* • press the ***Delete*** button in the ***Instruction box***, *or* • press the ***Delete*** key on your keyboard.

End_Block instruction

If you delete the ***End_Block*** instruction, the block will end at the last instruction in the block. If a gradient is currently being formed, the gradient will continue into the next block.

How to suspend execution temporarily

An instruction that has been deleted can only be recovered by re-inserting the instruction. If you want to suspend execution of an instruction temporarily (for example during development work), you can replace the breakpoint with a value after the ***End_Block*** or ***End_Method*** instruction.

6.3.4 How to change or move method instructions

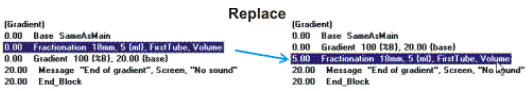
How to change an instruction

The table below describes how to change an instruction in the ***Text*** pane of the ***Text Instructions Editor***:

Step	Action
1	Select the instruction. *Result:* The instruction with its current parameters is displayed in the ***Instruction box***.
2	Make the required changes to the breakpoint or parameters *or* select a new instruction in the ***Instruction Box***.
3	Click the ***Change*** button *or* the ***Replace*** button. *Note*: These buttons are equivalent unless changes are made to the breakpoint or the length of a gradient. See below.

Effects of the Change button and the Replace button on breakpoints

The table below describes the difference in function between the ***Change*** button and the ***Replace*** button when you change breakpoints:

Button	Function
Change	This button shifts all subsequent instructions in the block according to the change in the breakpoint. ***Change*** does not affect the relative order of instructions in the method. You cannot change the breakpoint of an instruction to earlier than the nearest previous breakpoint in a block. The illustration shows an example where ***Fractionation*** is changed from breakpoint 0 to 5:
Replace	This button moves the selected instruction but does not change the breakpoint of any other instruction. ***Replace*** can change the relative order of instructions in the method. The illustration shows an example where ***Fractionation*** is changed from breakpoint 0 to 5: 

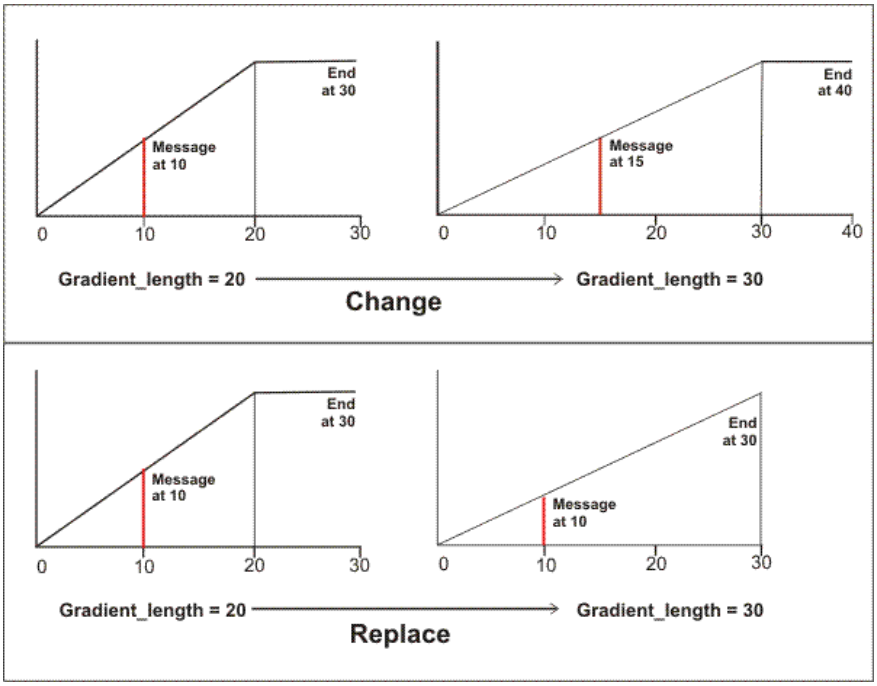
Effects of the Change button and the Replace button on gradient length

The ***Length*** parameter in the ***Gradient*** instruction affects the length of a gradient. Depending on which button you use, the change will have different results. The table below describes this:

Command	Function
Change	If this button is used to change the length of a gradient, the breakpoints for any instructions issued during the progress of the gradient will be adjusted proportionately so that they are always placed at the same relative position within the gradient. Instructions issued after the end of the gradient will be shifted by the amount of the change. Since the gradient works over time, any instruction that you want to insert after a gradient should be placed after the combined breakpoint and gradient length. *Note:* Moving the ***End_block*** instruction in a gradient block with the ***Change*** button does not affect the length of the gradient.
Replace	If this button is used to change the length of a gradient, other instructions are not affected.

Illustration of the effects of the Change button vs. the Replace button on gradients

The illustration shows the different effects of the ***Change*** button and the ***Replace*** button on instructions within and after gradients:



How to move an instruction

Move an instruction within the same breakpoint

Select the instruction in the ***Text*** pane of the ***Text Instructions Editor*** and drag it to its new location to change the order of instructions within the same breakpoint in a block.

Move an instruction to another breakpoint

The table below describes how to move an instruction to another breakpoint:

Step	Action
1	• Select the instruction in the ***Text*** pane of the ***Text Instructions Editor***. • Choose ***Edit:Cut***.
2	Select the instruction line just *above* the point where you want the cut instruction to be pasted. Choose ***Edit:Paste***. *Result:* The instruction is now removed from its original breakpoint and pasted at the new breakpoint. The pasted instruction is inserted with the same breakpoint value as the instruction selected for point of insertion.

6.4 How to use method variables

Introduction

Method variables can be used to edit suitable methods. Variables can be assigned to most instruction parameters including breakpoints. Variables also form the foundation for automatic method scouting.

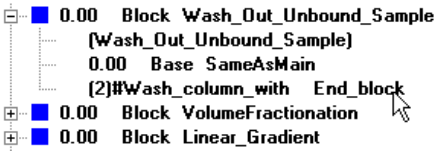
Each parameter defined as a variable is also assigned a default value, which is used if no changes are made to variable values at the start of a run. Up to 500 variables can be defined in a single method.

All variables are listed on the ***Variables*** tab of the ***Run Setup***, grouped according to the block in which they appear. See *Section 6.5.2 The Variables tab, on page 153*.

Identifying variables

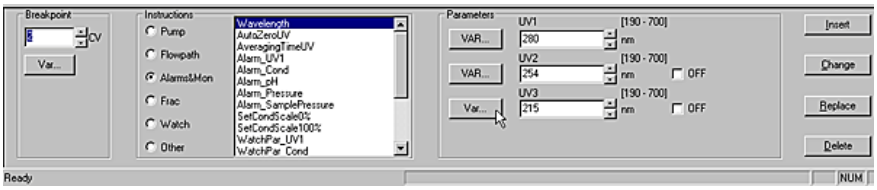
Parameters defined as variables can be identified in two ways:

- In the ***Text*** pane in ***Text instructions***, the parameter is given as the default value in parentheses followed by the variable name. The illustration below shows an example of this:



- When the instruction is shown in the ***Instructions*** field of the ***Instruction box***, the ***VAR*** button beside the parameter field is displayed in capital letters, that is ***VAR*** not ***Var***.

  The illustration below shows an example of the ***Instruction box*** where ***UV1*** and ***UV2*** are defined as variables and the ***UV3*** position is fixed.



When to change variable values

Variable values can be changed immediately before the start of a method run without using the ***Method Editor***, allowing one method to be used for runs under a variety of conditions.

How to change variable values

To change default variable values, you can either

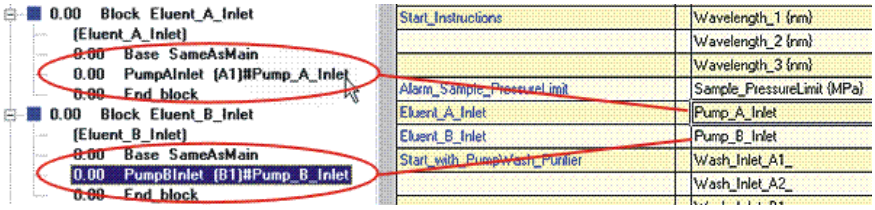
- edit the instruction in the ***Instruction box***

or

- change the value in the ***Variables*** tab of ***Run Setup***.

Changes made in the ***Text*** pane are automatically updated on the ***Variables*** tab and vice versa.

The figure below illustrates the relationship between variables in the ***Text*** pane and on the ***Variables*** tab of ***Run Setup***:



Breakpoints or gradient lengths

If a breakpoint or gradient length is defined as a variable, changing the variable value in the ***Variables*** tab when the method run is started will shift other instruction breakpoints accordingly. This functionality is equivalent to using the ***Change*** button to alter a breakpoint or gradient length (see *Section 6.3.4 How to change or move method instructions, on page 140* for how the ***Change*** button affects instructions within gradients).

How to define new variables

Only one variable that affects block length (breakpoint or gradient length) may be defined within each block. However, any number of parameters may be defined as variables within a block. The table below describes how to define a new variable.

Step	Action
1	Select the instruction where you want to define the variable in the ***Text*** pane of ***Text instructions***. *Result:* The parameters for the instruction are shown in the ***Instruction box***.
2	• Locate the breakpoint or the required parameter in the ***Instruction box***. • Click the ***Var*** button. *Result:* The ***Variable Name Definition*** dialog box opens.
3	• Enter a name for the variable. • Select the ***Visible in details only*** check box if you want to set the variable as a "details" variable. Detail variables only become visible on the ***Variables*** tab if the ***Show details*** check box is selected. This option is useful for hiding less important variables. • Click ***OK***. *Result:* The ***Var*** button changes to ***VAR*** to confirm the new variable. The variable is displayed in the ***Text*** pane.

Variable names

Variables are defined with names that can be explicit descriptions of the variable function, for example ***Sample_volume*** and ***Gradient_length***. Suitable choices of variable names can make the method easier to read and understand, and also help the operator in setting variable values at the start of a method run.

The names can be up to 32 characters long and the following characters can be used:

- Letters (A-Z)
- Digits (0-9)
- The underscore character (_)

The case of letters is retained, but not significant. The names ***Flow_Rate*** and ***FLOW_RATE*** are treated as identical.

How to rename a variable

The table below describes how to rename a variable:

Step	Action
1	Select the instruction that includes the variable you wish to rename in the ***Text*** pane of ***Text instructions***. *Result:* The parameters for the instruction are shown in the ***Instruction box***.
2	• Locate the required parameter in the ***Parameters*** field. • Click the ***VAR*** button.
3	Enter a new variable name in the dialog box and click ***OK***.

Note: Variables can also be renamed in the ***Edit Variables*** dialog box in the ***Method Editor***. See *Section 6.5.2 The Variables tab, on page 153* for more information.

How to remove a variable

The table below describes how to remove a variable by converting it into a fixed value:

Step	Action
1	In the ***Text*** pane of ***Text instructions***, select the instruction with the variable you want to remove. *Result:* The parameters for the instruction are shown in the ***Instruction box***.
2	• Locate the required parameter in the ***Parameters*** field. • Click the ***VAR*** button.
3	• Click the ***Clear*** button to delete the variable. • Click ***OK***. *Result:* The ***VAR*** button changes to ***Var*** to confirm that the variable is removed.

Note: Variables can also be deleted in the ***Edit Variables*** dialog box in the ***Method Editor***. See *Section 6.5.2 The Variables tab, on page 153* for more information.

6.5 Run Setup

Introduction

Run Setup is a part of the ***Method Editor***. It has several tabs for defining method properties. This section describes how to use the tabs and the information displayed on the tabs.

In this section

This section contains these topics:

Section	See page
6.5.1 Overview of Run Setup	150
6.5.2 The Variables tab	153
6.5.3 The Scouting tab	156
6.5.4 The Questions tab	157
6.5.5 The Gradient tab	161
6.5.6 The Notes tab	164
6.5.7 The Evaluation Procedures tab	166
6.5.8 The Reference Curves tab	171
6.5.9 The Columns tab	173
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6.5.11 The Method Information tab	178
6.5.12 The Result Name tab	180
6.5.13 The Frac-950 tab	183
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6.5.15 How to export the values in the Run Setup	187

6.5.1 Overview of Run Setup

Introduction

To access ***Run Setup***, either

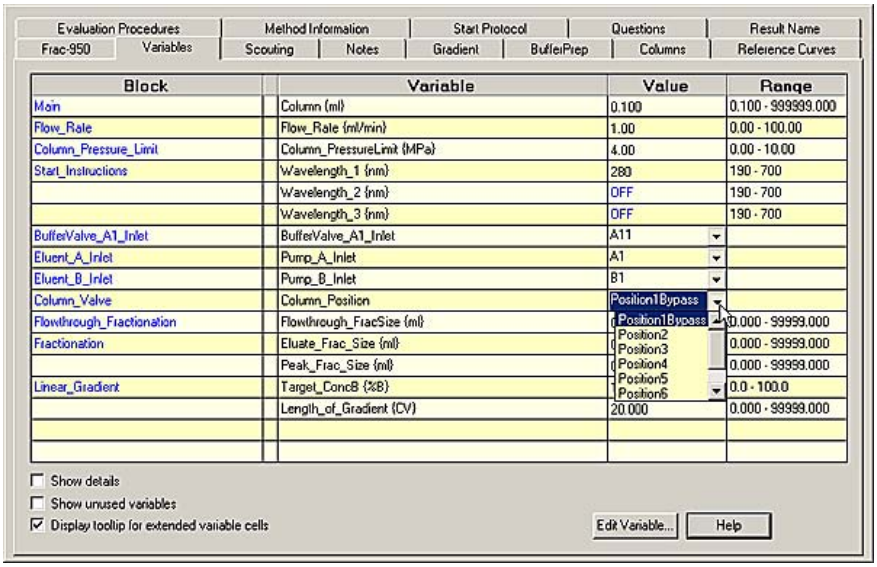
- Click the ***Run Setup*** icon on the ***Method Editor*** toolbar,

or

- Select ***View: Run Setup***.

Illustration of Run Setup

The illustration below shows an example of the ***Run Setup*** with the ***Variables*** tab selected:



The tabs

The table below contains brief descriptions of the tabs of ***Run Setup***. If you want more detailed descriptions, see sections on the respective tabs:

Tab	This tab...
Frac-950	allows the user to choose rack type and the fractionation order for the Frac-950 fraction collector.
Variables	lists all variables used in the method with their default values, organized by method block.
Scouting	shows the scouting scheme used for the method. The scouting scheme can also be set up from this tab. *Note*: Methods including scouting are only allowed on ÄKTAxpress systems if the UNICORN software has been installed in classic mode.
Notes	shows the descriptive comments that form a part of the method documentation.
Gradient	provides a graphical overview of the block structure and eluent gradient tab in the current method.
BufferPrep	displays information about the selected buffer preparation recipe for the current method.
Columns	displays the columns used in the current method.
Reference curves	displays the reference curves that will appear in the ***System Control curve*** dialog box during the run of the current method.
Evaluation Procedures	shows the evaluation procedures that will run at the end of the current method.
Method Information	displays information about the method, such as method name, target system, and last date of change.
Start Protocol	determines which items of the ***Run Setup*** that are displayed at the start of the run.
Questions	displays the questions used in the method. Questions provide a means for entering run-specific information at the start of a run. Use this tab when you want to define questions.

Tab	This tab...
Result name	specifies how the result files will be named for the results of a run, and where the result file will be saved.

6.5.2 The Variables tab

Introduction

The ***Variables*** tab lists all variables used in the method with their default values, organized by method block. You can change the default values to create a variant of the method.

Note: The variables of a block are only displayed once on the ***Variables*** tab, even if the block is called several times in a method. ***Variables*** are displayed only if the method contains variables.

Check boxes

There are three check boxes on the ***Variables*** tab. The table below describes these boxes:

Check box	Select this box if you want...
Show details	detail variables to be shown. Detail variables are indicated by a ***D*** in the column immediately to the left of the ***Variable*** column.
Show unused variables	unused variables to be shown. Unused variables are indicated by a ***U*** in the column immediately to the left of the ***Variable*** column.
Display tooltip for extended variable cells	to display useful tips when you move the cursor to fields that can have several functions.

Note: The options to show detail and unused variables can be set up as default options in the ***Administration:Change User Attributes*** settings in the ***UNICORN Manager***.

How to change the default values

Enter new values in the appropriate fields to change the default variable values. For some variables, pre-set values are available on drop-down menus. Save the method when you have made your changes.

Note: The ***Variables*** box must be selected on the ***Start Protocol*** tab if you want to be able to change variable values at the start of a method.

Blue values

For variables with values shown in blue, the value input can be toggled between ***OFF***, ***INFINITE*** or other single position values, and a variable range. To change the value, right-click the value cell.

Variables can also be changed in the Text Instructions Editor

Variables can be changed in the ***Text Instructions Editor*** as well as on the ***Variables*** tab of the ***Method Editor***. Changed values will be displayed for the corresponding instructions in both windows.

How to delete or rename variables

The table below describes how to delete or rename a variable in the ***Run Setup***.

Step	Action
1	• Click the ***Edit Variable...*** button on the ***Run Setup Variables*** tab. *or* • Choose the ***Edit:Variable... Method Editor*** menu option. *Result*: The ***Edit Variables*** dialog box opens. The variables are listed alphabetically.
2	Select the variable to edit.
3	**Rename** • Type a new variable name in the ***New name*** text box. • Click the ***Rename*** button. *Result*: The variable is renamed. **Delete** • Click the ***Delete*** button. • Confirm that you want to delete the variable. *Result*: The variable is deleted.

How to change a variable into a detail variable

Detail variables are only shown if the ***Show details*** checkbox is selected on the ***Variables*** tab. The table below describes how to set up a detail variable.

Step	Action
1	• Click the ***Edit Variable...*** button on the ***Run Setup Variables*** tab. *or* • Choose the ***Edit:Variable... Method Editor*** menu option. *Result*: The ***Edit Variables*** dialog box opens. The variables are listed alphabetically.
2	Select the variable to be changed.
3	• Select the ***Set visible in details only*** checkbox. • Click the ***Close*** button. *Result*: The variable is marked by the detail indicator ***D***.

How to change a detail variable into a regular variable

The table below describes how to change a detail variable into a regular variable.

Step	Action
1	• Click the ***Edit Variable...*** button on the ***Run Setup Variables*** tab. *or* • Choose the ***Edit:Variable... Method Editor*** menu option. *Result*: The ***Edit Variables*** dialog box opens. The variables are listed alphabetically.
2	Select the variable to be changed.
3	• De-select the ***Set visible in details only*** checkbox. • Click the ***Close*** button. *Result*: The detail variable indicator ***D*** is removed.

6.5.3 The Scouting tab

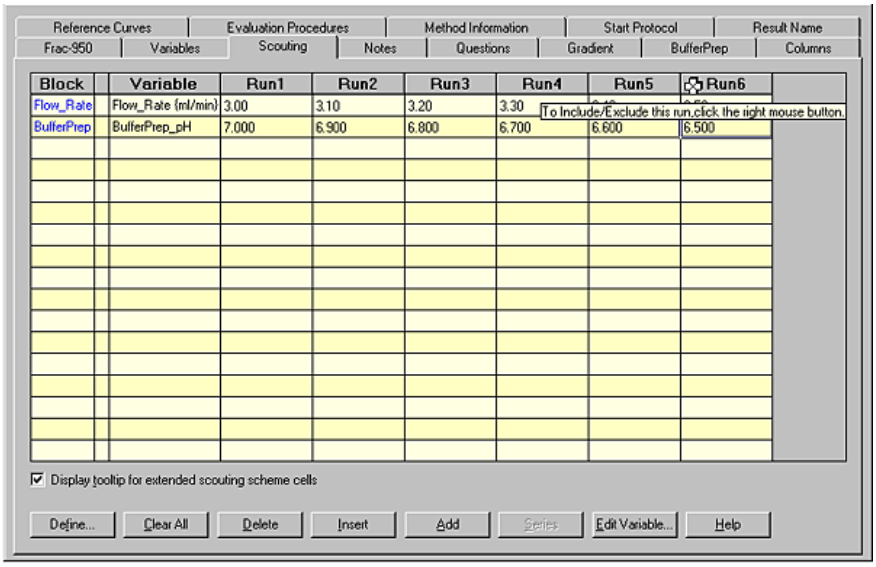
Introduction

A scouting scheme is a series of runs where chosen variable values are varied. You can define up to 99 runs in a scouting scheme. When a method is run with scouting, the method is automatically repeated for each selected run in the scouting scheme. Typically, scouting will vary one or more variables in a series of runs, for example, flow rate or elution gradient. See *Chapter 7 Scouting, on page 213* for instructions on how to set up a scouting scheme, and *Section 9.4 How to perform a scouting run, on page 260*

Note: The ***Scouting*** tab is available only if the method contains variables.

Example of a scouting scheme

The illustration below shows a scouting scheme for six flow rates and different pH values:



Note: The ***Edit Variable...*** button on the ***Scouting*** tab opens the same ***Edit Variables*** dialog box that can be accessed from the ***Variables*** tab.

6.5.4 The Questions tab

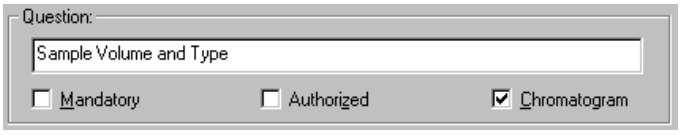
Introduction

The ***Questions*** tab of ***Run Setup*** is used for viewing and adding questions that the system asks a user at the start of a run. These questions provide a means for entering structured run-specific information. Method wizards and templates supplied with UNICORN are defined with a set of questions for sample, column and eluent identification.

Note: For questions to be shown in the start protocol, the ***Questions*** option must be checked on the ***Start Protocol*** tab of ***Run Setup***.

Question status

Different types of questions have different status. The illustration below shows the ***Question*** field, an example of a question and the status alternatives that can be used:

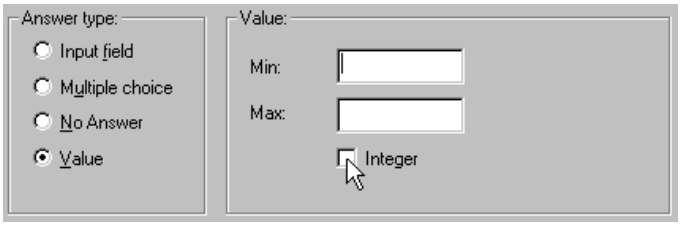


The table below explains the different alternatives:

Question status	Explanation
Mandatory	These questions must be answered before a method is started.
Authorized	These questions must be signed with the users signature password to unlock and continue the method.
Chromatogram	These questions will be printed with the answers on the same page as the chromatogram, if a question is chosen in an evaluation report.

Answer type

A question has to be defined to accept one of four types of answers. The illustration below shows an example where the ***Value*** option has been selected. The appearance of the box to the right of the ***Answer type*** field depends on the answer type option selected:



The table below describes the different answer types:

Answer type	This option...
Input field	accepts any alphanumerical input as the answer. Input field questions may have a default answer.
Multiple choice	allows the user to choose one of a defined set of answers. To allow a blank answer, enter a space in one of the pre-defined answers.
No Answer	is used to • display important information *or* • to split a question over more than one line by setting all but the last line in a question to ***No answer***. (Normally, each question consists of one line only.) It is impossible to give an answer to questions with this option selected.
Value	accepts only numerical answers. ***Value*** questions must have specified maximum and minimum limits, and may be defined to accept only integer values.

How to insert a question

The table below describes how to insert a question:

Step	Action
1	If there are questions on the list, select the question that should be followed by the new question.
2	Enter the question text, status, answer type and answer option as required.
3	The ***Answer type*** determines what is displayed in the question definition field to the right of the ***Answer type*** field. For each answer type, do as follows: **Input field** Enter a default answer if required. **Multiple choice** • Click in the text field under ***Alternatives***. • Enter the answer. • Click the ***Add/Delete*** button. *Result:* The new alternative is added at the end of the list. • Repeat this procedure to add new alternatives. To remove an alternative, mark the alternative in the scroll list and click the ***Add/Delete*** button. **No answer** No action taken. **Value** Enter maximum and minimum limits. Select the ***Integer*** box if the question is to accept integers only as answers.
4	Click the ***Insert*** button. Result: The new question is added to the list.

How to preview questions

The table below describes how to preview the questions as they will appear in the ***Start Protocol***.

Step	Action
1	• Select a question. • Click the ***Preview*** button. *Result*: The question is displayed.
2	Click the ***Edit*** button to return to the question editing mode.

How to edit a question

The table below describes how to edit a question:

Step	Action
1	Select the question you want to edit.
2	Change the text, status, type and answer as required
3	Click the ***Replace*** button.

How to delete a question

Do one of the following to delete a question:

- Select a question and click the ***Delete*** button to remove the selected question.
- Click the ***Delete all*** button to delete all questions.

6.5.5 The Gradient tab

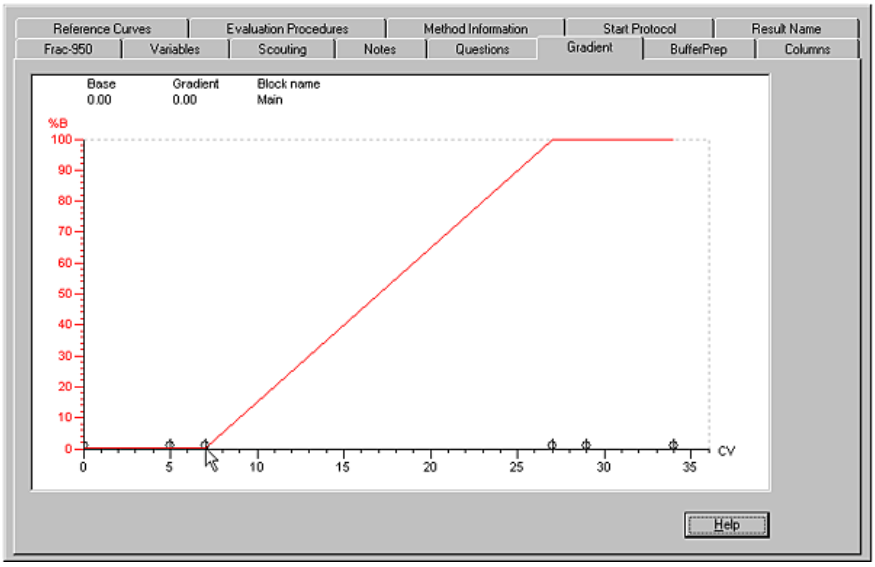
Introduction

The ***Gradient*** tab provides a graphical overview of the block structure and eluent gradient in the current method. The description of this tab can also serve as a description of the ***Gradient*** pane of the ***Text Instructions***.

Note: For scouting runs, click ***Run X*** to see the gradient for each run.

Illustration

The illustration below shows an example of a ***Gradient*** tab:



How to zoom in on a selected region

The table below describes how to zoom in on a selected area of the ***Gradient*** tab:

Step	Action
1	• Press and hold the left mouse button and drag a rectangle on the screen to select the area you want to zoom in on. • Release the mouse button. *Result:* The display is now zoomed in on the selected area.
2	Repeat the process for further magnification of selected areas.

How to reduce the scale of the zoom function

To reduce the scale of the zoom function, right-click the tab and choose either:

- ***Undo Zoom*** to reverse each zoom-in action a step at a time, or
- ***Reset Zoom*** to reverse all of the zoom-in actions to the default scale setting.

How to use the vertical marker line

A vertical marker line can be dragged from the Y-axis with the mouse. As you drag the marker line, the current position is identified at the top of the tab in terms of the block name, X-position in the currently displayed base and eluent concentration in per cent of eluent B.

How to change the base shown on the X-axis

You can change the base shown on the ***Gradient*** X-axis. The alternatives are time, volume and column volumes. Changing the base for the display does not affect the base in the method instructions, which means that you can check how long a method will take simply by setting the axis scale to time, even if the method blocks are written in volume or column volume base.

The list below describes two ways to change the base shown on the X-axis:

- Click the X-axis to toggle between the base types.

or

- Right-click anywhere on the ***Gradient*** tab.

  Result: A sub-menu is displayed.
- Select ***Base*** and make the appropriate choice: ***Time***, ***Volume*** or ***CV***.

How to view hatch marks

You can display a hatched background on the ***Gradient*** tab. The table below describes how to do this:

Step	Action
1	Right-click anywhere on the ***Gradient*** tab. *Result:* A sub-menu is displayed.
2	Select ***Hatch***. *Result:* The ***Gradient*** background is hatched.
3	To hide the hatch marks, repeat steps 1 and 2.

6.5.6 The Notes tab

Introduction

Notes are descriptive comments that form part of the method documentation. Method templates are supplied with notes describing the system requirements for running the method. Read through these notes carefully before using a method.

Sub-tabs

There are four sub-tabs:

- ***Method Notes***
- ***Start Notes***
- ***Run Notes***
- ***Evaluation Notes***

Only the ***Method Notes*** can be edited from the ***Method Editor***; the other notes are accessible at the respective stages in a run.

Recommended usage

We recommend that you use ***Method Notes*** to describe the system setup required by the method (for example eluent and sample inlets, outlets and column connections).

Use the ***Start Notes*** or ***Run Notes*** for run-specific information.

Note: ***Method Notes*** are saved with the method and apply to all runs made with the method.

How to write method notes

To write method notes in your own methods, place the cursor in the white area of the ***Notes*** tab and type the relevant text. Use standard Windows editing functions to edit the notes.

How to search for text strings

You can search for text strings in the method notes. The table below describes how to perform a search.

Step	Action
1	Click the ***Find*** button. *Result*: The ***Find*** dialog box opens.
2	• Type the text string in the ***Find what*** text box. • Select search criteria and click ***OK***. *Result*: The located text string is highlighted in the text area.

6.5.7 The Evaluation Procedures tab

Introduction

The ***Evaluation Procedures*** tab lists all evaluation procedures associated with the method. Evaluation procedures can be called automatically at the end of a method to evaluate and/or print the results.

Many UNICORN strategies are supplied with method templates or wizards that include a number of evaluation procedures. User defined procedures are created in the evaluation module and can be saved in method files (see *Section 12.3 Automated evaluation procedures, on page 460*).

Changes in the Evaluation module

A procedure in a method will not be updated when a procedure with the same name is changed in the ***Evaluation*** module. The same applies to report formats saved in a procedure.

References to curves

Evaluation procedures that process chromatogram data rely on consistent identification of curves in the result file for correct operation. If you include evaluation procedures with a method, make sure that references to curves in the procedure will be valid when the procedure is executed at the end of the run (see *Section 12.3 Automated evaluation procedures, on page 460* for more details).

How to print evaluation results

If you use an evaluation procedure to print results automatically from a run controlled from a remote station in a network installation, the results will be printed on the printer currently set up on the local station, not on the remote station.

If you execute the procedure interactively from the ***Evaluation*** module on the remote station, the results will be printed on the printer set up on the remote station where you are working.

How to define and view evaluation procedures

Evaluation procedures are defined in the ***Evaluation*** module.

Procedures imported to a method can also be viewed and edited in the ***Method Editor***. To do this, select the required procedure on the list and click the ***Edit*** button.

How to select procedures to run

To select procedures to run, select the procedure(s) that are to be executed at the end of the run. The procedures will be executed in the order they appear on the list.

How to import evaluation procedures

The table describes how to import global evaluation procedures:

Note: Procedures saved with one method file can be imported to another.

Step	Action
1	Select the ***Evaluation Procedures*** tab and click the ***Import*** button. *Result:* The ***Import*** dialog box is displayed.
2	Choose either option 1 or 2 below. **Option 1: Select a global UNICORN procedure** 1 Select a procedure on the ***Select*** list. *Result:* The evaluation procedure name is displayed in the ***Import as*** field. **Option 2: Select a procedure from another method** 1 Select a method, that contains a procedure, in the left part of the dialog box. *Result:* The procedures of the selected method will be displayed on the ***Select*** list. 2 Select the desired procedure on the ***Select*** list. *Result:* The method name is displayed in the ***Import as*** field. *Note:* Click ***Procedure List*** to return to the list of UNICORN's global evaluation procedures.

Step	Action
3	If desired, change the procedure name in the ***Import as*** field. *Note:* The imported evaluation procedure cannot have the same name as an existing evaluation procedure in the method. If the default name is not allowed for this reason, the ***Import*** button will be gray and disabled. When you change the name in the ***Import as*** field, the button will become available again.
4	Click the ***Import*** button. *Result:* The evaluation procedure is imported into the method.
5	Repeat steps 2 - 4 until you have imported all procedures.
6	Click the ***Close*** button.

How to delete evaluation procedures

The table describes how to delete evaluation procedures from the method:

Step	Action
1	Select the ***Evaluation Procedures*** tab.
2	Select the procedure(s) that you want to delete.
3	Click the ***Delete*** button and confirm the deletion when prompted. *Result*: The deleted procedures are immediately removed from the method file.

How to rename evaluation procedures

The table describes how to rename evaluation procedures in a method.

Step	Action
1	Select the ***Evaluation Procedures*** tab and click the ***Rename*** button. *Result:* The ***Rename*** dialog box is displayed.

Step	Action
2	• Select a procedure from the list and change the name in the ***Rename item to*** field. • Click ***Rename***.
3	Repeat step 2 until you have renamed all procedures required.
4	Click the ***Close*** button.

How to edit an evaluation procedure

The table describes how to edit evaluation procedures in a specific method:

Step	Action
1	Select a procedure on the ***Evaluation Procedures*** tab and click the ***Edit*** button. *Result:* The ***Procedure Editor*** dialog box is displayed, with information about the selected procedure.
2	Enter the new parameter values in the appropriate place of the ***Parameters*** field, and click the ***Replace*** button. *Result:* The selected instruction in the evaluation procedure is updated in accordance with the new parameters assigned to it.
3	If needed, insert new instructions after the currently selected procedure instruction. Do the following: 1 Select an instruction type and instruction in the ***Instructions*** field. 2 Enter the appropriate parameter values in the ***Parameters*** field. 3 Click the ***Insert*** button. *Result:* The new instruction is added to the evaluation procedure.
4	To remove an instruction from the evaluation procedure, select it and click the ***Delete*** button.
5	Select ***File:Save as*** to save the edited procedure with a new name. Click the ***Close*** button.

Step	Action
6	Select ***File:Close*** from the menu in the ***Procedure Editor*** dialog box. *Result:* The ***Procedure Editor*** dialog box is closed and the procedure is saved automatically.

6.5.8 The Reference Curves tab

Introduction

Reference curves are curves from existing result files that you can display in the ***Curves*** pane of ***System Control*** during a run.

How to choose and display reference curves

You can include up to five reference curves in a method. You choose which curves to display during the run with the ***View:Properties:Curves*** command in ***System Control*** (see *Section 9.2.3 The Curves pane, on page 240*). Reference curves are only displayed during the run. Reference curves are not saved in the result file.

Note: Although this function can be used it is normally not useful for oligo applications.

How to add reference curves

The table below describes how to add a reference curve from a result file:

Step	Action
1	Select the ***Reference Curves*** tab and click the ***Import*** button. *Result:* The ***Import Reference Curve*** dialog is displayed.
2	• In the left field, select the result file containing the curve to be added. *Result:* The ***Select*** list displays the available curves for the result file. • Select the curve you want to add from the ***Select*** list.
3	• If desired, change the curve name in the ***Import as*** field. *Note:* The curve name has to be changed if a reference curve with that name already exists. • Click ***Import***.
4	Repeat steps 2 and 3 if you want to add more curves.
5	Click the ***Close*** button to close the ***Import Reference Curve*** dialog box.

How to delete reference curves

The table describes how to delete reference curves.

Step	Action
1	Select the curves you want to delete.
2	Click the ***Delete*** button and confirm the action when prompted.

Note: Deleting curves from the method does not affect the curves in the result file from which they were imported.

How to rename reference curves

The table below describes how to rename a reference curve in a method:

Step	Action
1	Click the ***Rename*** button.
2	• Select a curve from the list. • Change the name in the ***Rename item to*** field. • Click the ***Rename*** button.
3	Repeat steps 2 and 3 if you want to rename more reference curves.
4	Click the ***Close*** button. *Result:* The reference curve name is changed.

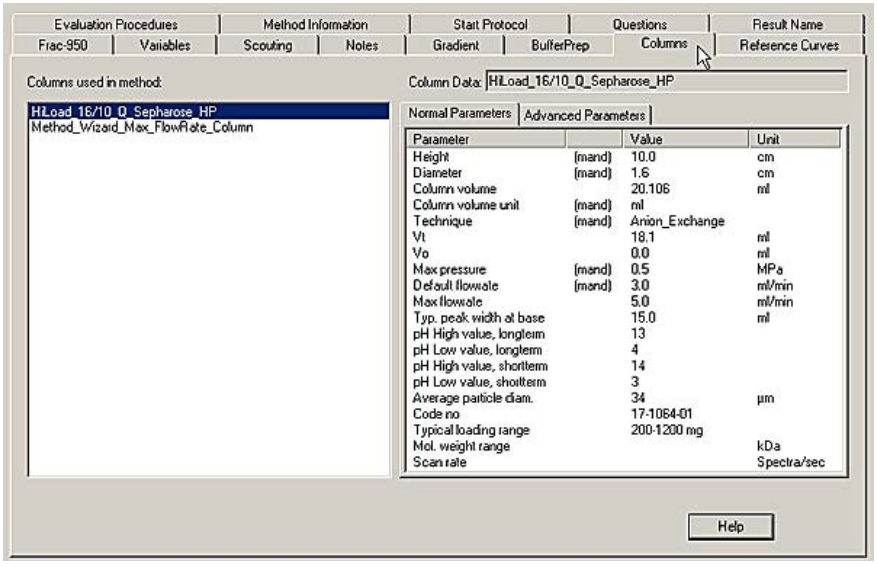
6.5.9 The Columns tab

Display of the column parameters

The ***Columns*** tab shows the parameters of the column selected for your method. The column parameters are displayed in the ***Column Data*** field. If you perform scouting runs with different columns, all of these will be listed. Select the appropriate column to display the parameters.

Illustration

The illustration shows an example of the ***Columns*** tab:



6.5.10 The BufferPrep tab

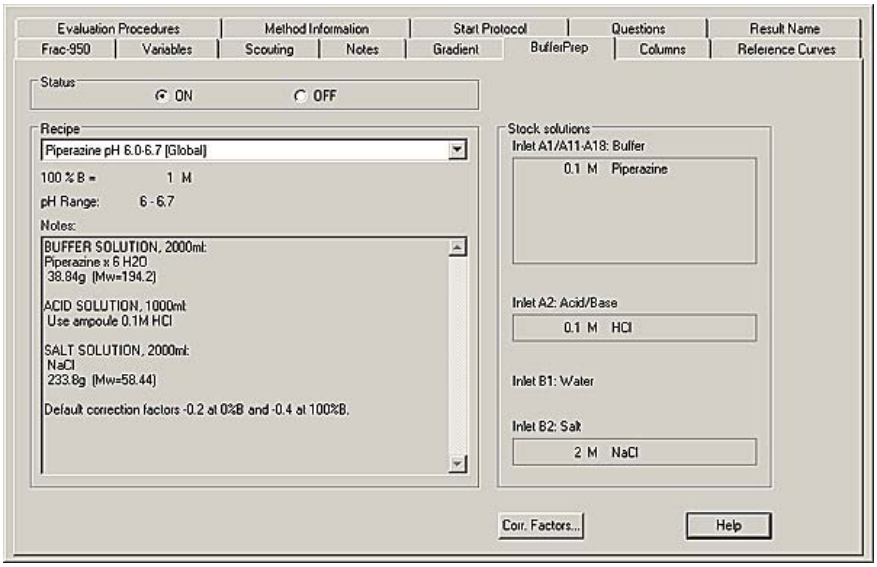
BufferPrep usage

BufferPrep allows a buffer of different pH and salt concentrations to be prepared on-line from four stock solutions. This removes the need to manually prepare new buffers every time the pH needs to be changed. Linear and step salt gradients can be run and pH can be used as a variable scouting parameter. ***BufferPrep*** is optimized for cation and anion exchange chromatography. For a complete description of ***BufferPrep***, see the user manual for ÄKTAdesign systems.

Note: ***BufferPrep*** is only available for some ÄKTAdesign systems.

Illustration

The illustration below shows an example of the ***BufferPrep*** tab:



Stock solutions

The solutions and the inlets to which they should be connected are displayed to the right of the dialog box. Accuracy of preparation is essential. The four stock solutions consist of:

- a mix of buffering components (there can be up to five different buffering components enabling a broad pH range to be covered),
- an acid (HCl) or base (NaOH) for pH on-line titration,
- distilled water,
- an inert salt (for example NaCl) for salt gradient formation.

How to create a BufferPrep method

If a suitable template or wizard is not available, you can create a ***BufferPrep*** method yourself. The instruction ***BufferPrep_pH*** must be available at breakpoint zero at the beginning of the method. The method must not contain the instructions ***PumpAInlet*** or ***PumpBInlet***.

The table shows one way to create a ***BufferPrep*** method.

Step	Action
1	In the ***Text Instruction*** editor: • Insert a ***BufferPrep-pH*** block at breakpoint zero at the beginning of the method. • Define ***BufferPrep-pH*** as a variable.
2	Change to the ***Run Setup***. • Select the ***BufferPrep*** tab. • Click the ***ON*** radio button in the ***Status*** field. • Select a ***Recipe*** from the drop-down list box. There are two main alternatives: - AIEX or CIEX, which are recipes covering a broad pH range, - single buffer recipes for more narrow pH ranges. *Result:* All information relevant to the selected recipe will be displayed on the tab.
3	Prepare the required stock solutions.

Step	Action
4	Do one of the following: • Select the ***Variables*** tab. Set the required pH for the method run in the variable ***BufferPrep_pH***, *or* • If you want to perform pH scouting, click the ***Scouting*** tab and select ***BufferPrep_pH*** as a scouting variable. Enter the pH values for the different runs.

BufferPrep recipes

The recipe saved in the method (the one selected on the ***BufferPrep*** tab) cannot be edited, although fine tuning is possible. However, the recipes on the list of all ***BufferPrep*** recipes can be edited. New recipes can also be created (see *Appendix E How to create and edit BufferPrep recipes, on page 638*).

How to fine tune the BufferPrep recipe with correction factors

In order to obtain high pH accuracy, the recipe can be fine tuned around a specific pH by setting correction factors. The table below describes how to fine tune the recipe with correction factors:

Step	Action
1	In ***System Control***, select ***Manual: Other***.
2	Select ***BufferPrep Recipe*** and ***Recipe Name***. Click the ***Execute*** button.
3	• Set the pH in the instruction ***BufferPrep_pH*** in group ***Pump***. • Click the ***Execute*** button.
4	• Set the flow rate to be used during the run in the ***Flow*** instruction. • Click the ***Execute*** button.
5	Check the pH reading when stable. Allow at least 30 ml of eluent to pass through before expecting a steady pH reading.

Step	Action
6	• Change to 100% B by setting the Gradient instruction in ***Manual:Pump*** to 100% for ***Target*** and 0 for ***Length***. • Click the ***Execute*** button.
7	Check the pH reading when stable at 100% B.
8	• If the readings are acceptable at both 0% and 100%, the correction factors do not need to be changed. • If the readings are not acceptable, click the ***Corr. Factors*** button in the ***BufferPrep*** tab in the method.
9	Enter the deviation at 0% and 100%. (e.g., if the pH is set to 7.0 and the actual pH is 7.1 enter 0.1. Enter -0.1 if the pH is 6.9). *Note:* If correction factors already exist, the measured pH deviation should be added to the old factors.
10	Save the method.

Note: When changing the correction factors for the recipe selected in the method, the recipe with the same name on the list of all ***BufferPrep*** recipes is not affected. The changes will only apply in the specific method.

6.5.11 The Method Information tab

Introduction

The ***Method Information*** tab displays information about the method. This tab is for information only and cannot be edited.

There are three sub-tabs on this tab: ***Information***, ***Signatures***, and ***Method duration***.

The Information sub-tab

The ***Information*** sub-tab displays

- method information such as method name, creation date, creator and date of last change,
- target system,
- strategy information such as strategy name, date and size.

The ***Strategy Notes*** button displays what systems, programs and file versions the strategy is designed for.

The Signatures sub-tab

The ***Signatures*** sub-tab has five information fields for all signatures. The table below describes the content of each field:

Field	Description
Date	Date of the signature.
Meaning	Short description explaining the meaning behind the signature.
User Name	User name of the user who signed the method.
Full Name	Full name of the user who signed the method.
Position	Position of the user.

The Method Duration sub-tab

The ***Method Duration*** sub-tab presents

- the estimated total time
- the estimated buffer volume required for the method.

If the method includes a scouting scheme, click the ***Run 'x'*** button to see values for the different scouting runs.

6.5.12 The Result Name tab

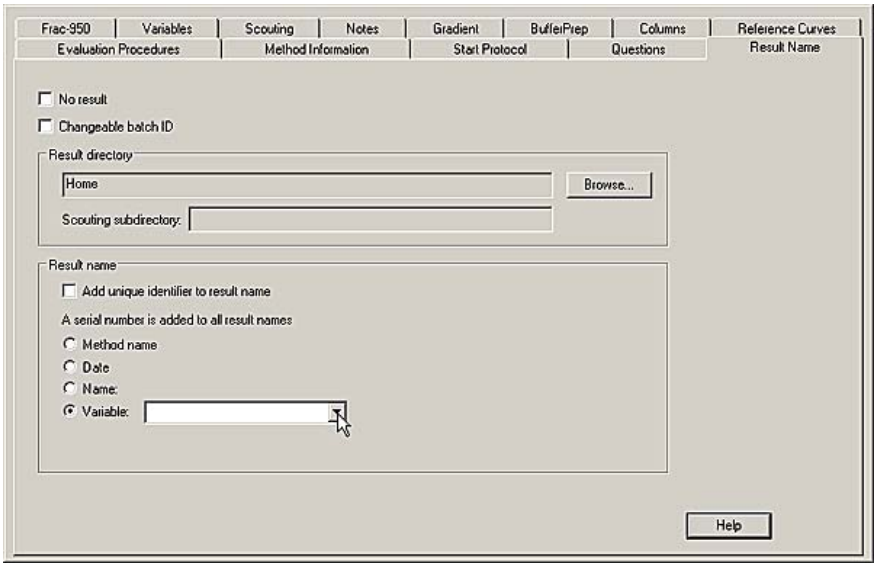
Introduction

The ***Result Name*** tab is used to specify:

- how the result files will be named for the results of a run
- where the result file will be saved
- the name of the special scouting folder where results from scouting runs will be stored.

Illustration

The illustration below shows an example of the ***Result Name*** tab:



Construction of the result file name

The result file name is constructed by one of the base options listed below. The serial number is changed automatically each time the method is run.

Base options of the result file name are:

- The ***Method name*** plus a 3-digit serial number,
- The ***Date*** of the run (in an 8-digit format determined by the country setting in Windows XP or Windows 7) plus a 3-digit serial number,
- A freely specified ***Name*** (within the file naming restrictions of the operating system) plus a 3-digit serial number.
- A selected ***Variable*** (from the droplist) plus a 3-digit serial number.

Note: If a result names includes decimal points (e.g. numeric variables) or underscore characters, these characters will automatically be replaced by spaces. Points and underscores are not allowed in the result names.

Serial numbers and unique identifiers

If the result file folder already contains files with the same file name base, the serial number is changed automatically. For scouting runs, the 3-digit serial number will be the number of the executed run column in the scouting scheme.

A unique identifier can also be generated automatically, in addition to the serial number. The identifier is a string of numbers inserted between the result file name and the three-digit serial number.

- Select ***Add unique identifier to result name*** in the ***Result*** name field.

Batch ID for each test run

UNICORN will automatically issue a ***Batch ID*** to each method run. This ID is displayed before the ***Base*** in the logbook and can be used to identify individual runs. See illustration in *Section 9.2.5 The Logbook pane, on page 249*. If ***Changeable batch ID*** is selected, another ID string can be typed in the ***Start Protocol***.

Specify result name as changeable

The result name can be specified as changeable in the ***Start Protocol*** (see *Section 6.5.14 The Start Protocol tab, on page 185*). In that case, the information you supply on the ***Result Name*** tab will be the suggested result name, but you can change this at the start of the run.

How to save the result files in a different folder

By default, result files are stored in the home folder of the user who starts the run. The table below describes how to change the folder where the result file will be stored:

Step	Action
1	If the run contains information that is not important, you can save disk space by selecting the ***No result*** check box, thereby storing the result in the ***Temporary*** folder (named ***Manual Runs***, where only the latest 10 result files are saved). If not, go to step 2.
2	Click the ***Browse*** button.
3	• Double-click the required folder icon. • Click the ***OK*** button.

How to save scouting results

Scouting results will be saved in a special folder as specified by the result file path. To select a folder, type a name for the folder in the ***Scouting*** subdirectory field. Each time the scouting method is run, a new folder will be created with the name and a serial number (entering IEXSC will create folders IEXSC001, IEXSC002, etc.).

Note: Scouting is only possible for ÄKTAxpress systems when the UNICORN software has been installed in classic mode.

6.5.13 The Frac-950 tab

Introduction

The ***Frac-950*** tab is used for defining options for ***Frac-950***. The user can choose rack type and fractionation order.

How to set up fractionation

The table describes how to set up the fractionation.

Step	Action
1	Select rack type from the ***Rack*** drop-down list.
2	Select the order for fractionation by using the ***Fraction order*** radio buttons.

Manual runs

In ***System Control***, for manual runs, the ***Frac-950*** tab cannot be used. Instead, use the manual fractionation instructions, starting with ***Man_***.

- Choose ***Manual:Frac*** to open the ***Frac Instructions*** dialog box.

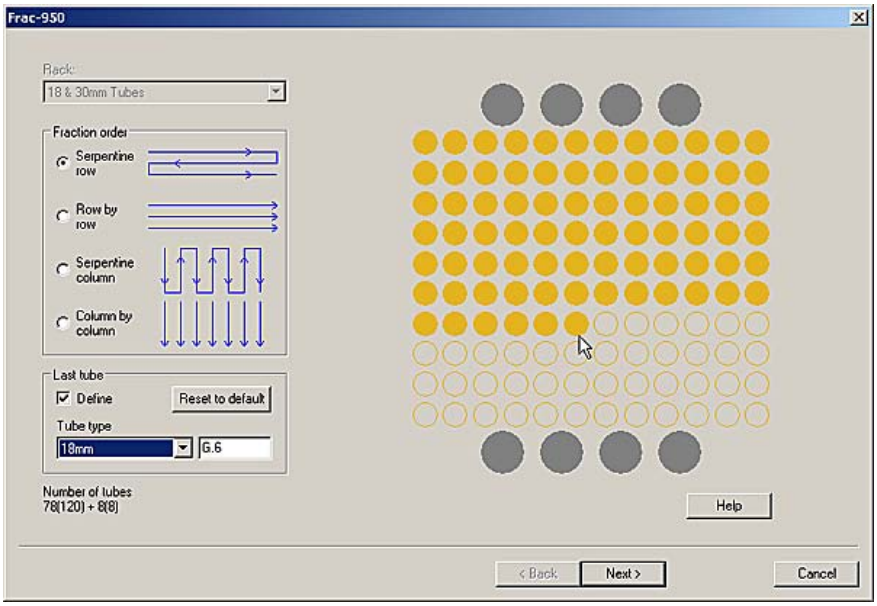
Total number of tubes

The total number of tubes sampled may differ if a last tube has been chosen. The ***Number of tubes*** equation in the bottom left corner of the ***Frac-950*** dialog box of the ***Start Protocol*** shows the current number of available tubes chosen for fractionation, followed by the total possible number in parentheses.

How to select the last tube

You can select a position for the last tube to be used in the fractionation process. If the process attempts to go further than the selected last tube during a method run, an alarm will be executed.

The last tube position can only be selected on the ***Frac-950*** dialog box in the ***Start Protocol*** when you start a method run, or when you do an instant run. The illustration below shows an example of this dialog box:



The lower right box within the ***Last tube*** field shows the currently selected last tube. The table below describes how to re-define the last tube:

Step	Action
1	In the ***Frac-950*** dialog box, select the ***Define*** box in the ***Last tube*** field to select the last tube position.
2	Place the cursor over the appropriate tube (circle) within the tube matrix and click again.

Note: When using different sized tubes in the same rack, the last tube can be set for both tube sizes. Use the ***Tube type*** drop-down list to choose the desired tube size, and then follow the procedures outlined above to select the last tube.

How to set the last tube to default setting

If you want to return to the default last tube position, click the ***Reset to default*** button of the ***Frac-950*** dialog box in the ***Start Protocol*** when you start a method run.

6.5.14 The Start Protocol tab

Introduction

The ***Start Protocol*** tab determines which items of the ***Run Setup*** are displayed at the start of a method run. Click the ***Start Protocol*** tab and select the items that you want to be displayed.

Checkboxes

The table below describes the check boxes of the ***Start Protocol*** tab:

Checkbox	Displays...
Frac-950	the ***Frac-950*** setup parameters, which can be changed.
Variables	values for method variables that can be changed at the start of the run. These values will override the default values for the particular run and be saved in the result file. The default values stored in the method are not affected.
Scouting	the scouting scheme which can be changed at the start of the run. Changes will override the default settings and values for the particular run and be saved in the result file. *Note*: Methods including scouting are only allowed on ÄKTAxpress with installations where classic mode was selected.
Text Method	method instructions. They cannot be changed from this display.
Notes	the ***Notes*** tab.
Gradient	the gradient.
BufferPrep	the recipe selected in the method. The recipe cannot be changed during the start of a run.
Columns	the available column definitions.
Reference curves	the reference curves associated with the method.

Checkbox	Displays...
Evaluation procedures	the evaluation procedures set to be executed at the end of the method.
Method information	the method information.
Settings	the settings.
Calibration	the monitor calibration settings.
Questions	questions defined in the method.You are recommended to always use this option, since the answers to questions can form an important part of the UNICORN run documentation.
Result name	the result name, which is changeable if this option has been selected. Click the ***Browse*** button to change the result folder. If the box is not selected, the result name will still be displayed, but you will not be able to change the name or folder.

Scouting start protocol field

The table below describes the options in the ***Scouting start protocol*** field.

Option	If you check this option...
First run only	parameters for the scouting runs can be adjusted at the beginning of the first run only. After that, the runs will be performed automatically without operator intervention.
All runs	the ***Scouting start protocol*** will be displayed at the beginning of each run in the scouting scheme.

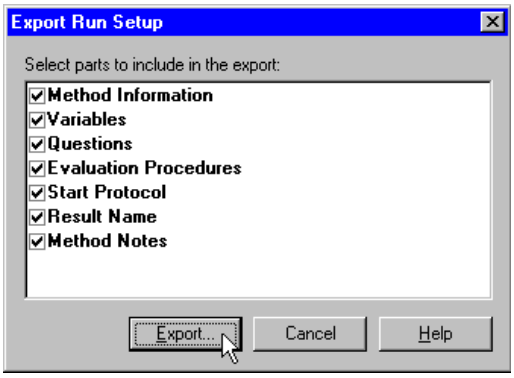
Note: Scouting is only possible on ÄKTAxpress systems where the UNICORN installation has been made in classic mode.

6.5.15 How to export the values in the Run Setup

Instruction

You can easily export the values in the ***Run Setup*** to a file, and save it in ASCII format. This is useful when you want to enable others to read the methods without having access to UNICORN on their computers.

The table below describes how to export the values in the ***Run Setup*** and save them to a file.

Step	Action
1	In the ***Text instructions Editor*** or the ***Run Setup***, select ***File:Export:Run Setup***. *Result:* The ***Export Run Setup*** dialog box is displayed. 
2	• Select the boxes to select the parts of ***Run Setup*** that you want to export. • Click the ***Export*** button. *Result:* The ***Export*** dialog box is displayed.
3	• Type a file name and select the target drive and folder. • Click the ***Save*** button.

6.6 How to use selected method instructions

Introduction

This section provides recommendations for how to use some common programming features in UNICORN methods. They are available from the ***Instruction box*** in the ***Method Editor***.

In this section

This section contains these topics:

Section	See page
6.6.1 Base instruction	189
6.6.2 Instructions at the same breakpoint	192
6.6.3 Block and method length	193
6.6.4 Messages and Set_Marks	195
6.6.5 How to delay a method	197
6.6.6 Linear flow rates	198
6.6.7 Gradients and eluent concentrations	199

6.6.1 Base instruction

Bases

Every method block must start with a ***Base*** instruction, defining the base for calculating breakpoints.

Different blocks can use different bases. The base can be one of the following:

- ***volume*** (the unit depends on the scale defined in the system strategy)
- ***time*** (minutes)
- ***column volume***, CV (defined as a numerical value or taken from the column definition)
- ***SameAsMain*** (all blocks apart from the main block), which means that the block will inherit the base defined in the main block.

Method blocks that use a volume or column volume base

Make sure that the flow rate is not zero. Volume breakpoints are calculated from the flow rate of the pump, and the method will not progress if the flow rate is zero.

What base should I use?

Use the base that most closely suits the purpose of the block. Column volume is recommended as the base for most steps in a run. In some situations, however, it may be more suitable to use a time or volume base for individual blocks.

To change the base for an existing method

Be careful when changing the base for an existing method. Changing between time and volume bases can affect the relative duration of steps in the method if different steps use different flow rates.

Column parameter: named column

If a named column is selected for the ***Column*** parameter in the ***Other:Base*** instruction, the volume specified in the selected column definition will automatically be used for column volume in the method block. The column volume for base ***CV*** cannot then be changed in the instruction or defined as a variable. However, the ***Column*** parameter should be defined as a variable. Choosing a column definition also enables linear flow rate and column performance calculations.

Column parameter: Any

If the ***Column*** parameter in the ***Other:Base*** instruction is set to ***Any*** and the ***Base*** parameter is set to ***CV***, the column volume is set numerically by the ***Volume*** parameter. The column volume may be defined as a variable, allowing the scale of the run to be decided when the method is actually run.

How to select columns for a template or wizard

In cases where a template or wizard-generated method and column are chosen, it is easy to select other columns for that method on the ***Variables*** tab in ***Run Setup***.

Note: This might not be possible for methods that you have created yourself.

How to select columns for a method not selected from a template

The table below describes how to select columns for a method, not selected from a template.

Step	Action
1	In the ***Instruction box*** of the ***Text instruction*** dialog box, mark the ***Other:Base*** instruction.
2	• Select the required column from the drop-down list for the ***Column*** parameter. • Click the ***Var...*** button to define the ***Column*** parameter as a variable. This is an optional but recommended step that will make it easy to change the column selection for different runs.
3	• Enter a variable name and click ***OK***. • Click ***Yes*** to confirm.

Column definition

A column definition can be chosen and defined as a variable even if the base for the block is set to volume or time. Parameters in the column definition will then be used for linear flow rate and column performance calculations.

Recommendation

A selected column definition applies locally within the block for which it is selected, and is not transferred to other blocks. We strongly recommend that the column definition be selected for the main block.

Update parameters

If you want parameters (for example, flow, pressure and averaging time) to be updated when you change the column, you must define these as variables.

Pump:Methodbase instruction

Volume or column volume base is calculated from the flow rate of the ***SystemPump*** or the ***SamplePump***, selected with the instruction ***Pump:Methodbase***. If no ***Pump:Methodbase*** instruction is included in the method, the default setting ***SystemPump*** will be used.

6.6.2 Instructions at the same breakpoint

Description

Instructions placed at the same breakpoint in a block are executed simultaneously.

Exceptions

Exceptions are successive ***Block*** instructions, which are executed in the sequence in which they are written. This can have important consequences in some situations.

The instruction sequence below shows an example of instructions with the same breakpoint, where the ***AutoZero_UV*** will start *after* the ***Wash*** block is completed.

Breakpoint	Instruction
0.00	Block WASH
0.00	AutoZero_UV
0.00	Block ELUATE

6.6.3 Block and method length

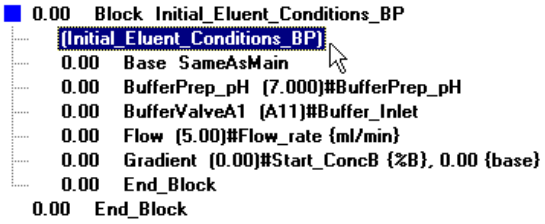
General description

The time or volume of a method run is determined by the sum of the block lengths. In turn, the length of a block is determined by the breakpoint of the last instruction in the block.

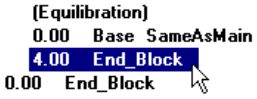
Note: Depending on how conditional calls are used (see *Section 6.7 Standard Watch conditions, on page 202*), the overall method time or volume may vary according to watch events during the run.

Block length

A block in which all breakpoints are set to 0 will take no time or volume during a method run. The illustration below shows an example of this:



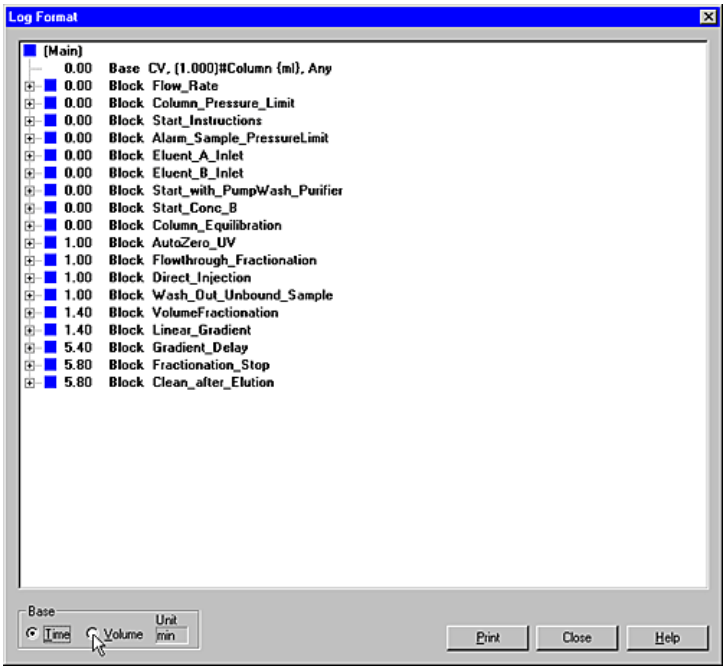
To extend the length of a block without performing any other operation, set the breakpoint of the ***End_block*** instruction appropriately, for example, as in the illustration below:



How to view the accumulated method time or volume

The Log Format window in the ***Method Editor*** shows the accumulated method time or volume for the current method. The accumulated time/volume is an approximation and does not take into account time or volume for ***Watch*** blocks, ***Wash*** commands or programmed ***Hold***. Also it does not compensate for splitter flow.

The table below describes how to view the accumulated method time or volume:

Step	Action
1	Select ***View:Log Format*** *or* click the ***Log Format*** icon. *Result:* The ***Log Format*** dialog box is displayed. 
2	If the method is a scouting run, click ***Run X*** to move between runs. *Note*: Scouting is only possible for ÄKTAxpress systems if the UNICORN software was installed in classic mode.

6.6.4 Messages and Set_Marks

When to use a message

Messages are used to inform the operator of the progress of the run. It is a good idea to issue messages at critical points in the method, for example, when ***Watch*** instructions are used for conditional events.

How to add a Message instruction

The ***Message*** instruction can be used to set up a message that will be displayed for the user during the execution of the method run. The message can be for information in a screen only, or it can require a signature before the user can control the system. The messages are all added to the logbook text. See *Section F.6 Messages, on page 660* for examples.

The table below describes how to add a ***Message*** instruction to the method.

Step	Action
1	• Select ***Other*** in the ***Instructions*** field of the ***Instructions box***. • Select ***Message*** in the instructions list.
2	Type a message in the ***Message*** text box in the ***Parameters*** field.
3	Select one of the display options on the ***Mode*** menu: • ***Screen***, i.e. only a text message is displayed. • ***Noscreen***, i.e. the message will not be displayed but only inserted into the logbook. • ***Authorize***, i.e. the message will require a signature from the user before the user can interact with the system again.
4	• Select a sound on the ***Sound*** menu if desired. • Click the ***Insert*** button.

Note: If the ***Message*** instruction is inserted in a conditional block it will only be displayed if the conditions of the block (for example a ***Watch***) is fulfilled.

Note: All messages are erased when the system reaches the ***End*** status. This also includes ***Authorize*** messages.

When to use a Set_Mark

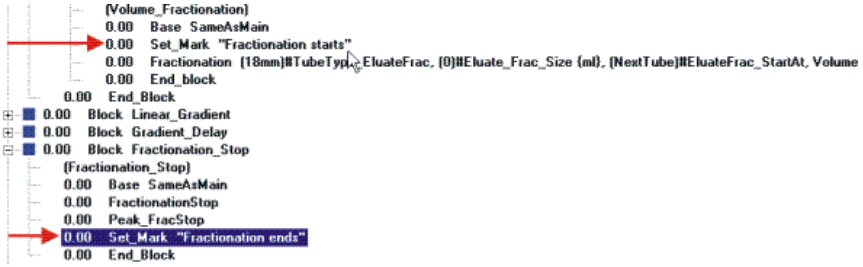
Set_Mark instructions are useful text messages. They can be used

- to insert manual notes, for example, when a problem occurs in a run
- to highlight certain stages in a method.

Set_Marks differ from ***Messages*** in that they are inserted into the chromatogram at set points as well as into the logbook during a method run.

Example of a Set_Mark

The illustration below shows an example where ***Set_Marks*** are used to highlight the start and end of fractionation in a method:



How to issue a Set_Mark

Set_Marks are issued from the ***Instructions box*** of the ***Text Instructions*** editor. The table below describes how to do this:

Step	Action
1	Select ***Other:Set_Mark*** in the ***Instructions box***.
2	Type the message in the ***Mark text*** field.
3	Click the ***Insert*** button. *Result:* A new line with the ***Set_Mark*** is added to the text instruction.

6.6.5 How to delay a method

Introduction

A method can be programmed to be delayed at critical points. There are three instructions for this purpose: ***Hold***, ***Pause*** and ***Hold_Until***. These instructions are described below.

Hold

The ***Hold*** instruction suspends the execution of the method, but continues to pump eluent at the current flow rate and concentration settings. For example, this instruction is useful for giving the operator time to load a sample loop.

Resume the method

The method may be resumed if you click ***Continue*** on the ***System Control*** toolbar.

Pause

The ***Pause*** instruction suspends execution of the method and stops the pumps so that the system comes to a standstill. In ÄKTAdesign systems valves remain in the position they were in before the pause. The pause may be defined as indefinite or for a given number of minutes. This instruction is most useful for stopping the system in the event of an unexpected condition.

Resume the method

The method may be resumed if you click ***Continue*** on the ***System Control*** toolbar.

Hold_Until

The ***Hold_Until*** instruction is a special kind of ***Watch*** instruction. The method is put on hold until a specific condition is met (signal, test or value) or the time-out is reached. Thereafter the remaining instructions in the method are executed.

Instructions that share the same breakpoint as the ***Hold_Until*** instruction, but are placed after it in the method, will be executed after the ***Hold_Until*** conditions have been met.

6.6.6 Linear flow rates

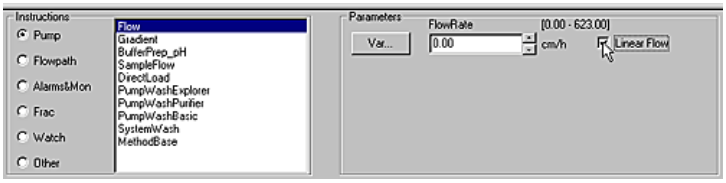
Introduction

Linear flow rates (cm/h) can be specified for ***Flow*** instructions. The volume flow rate is calculated from a specified linear flow rate and the column diameter as given in the column definition.

How to use linear flow rates

The table describes how to use linear flow rates.

Step	Action
1	Select a specific column on the ***Variables*** tab of the ***Run Setup***, *or* Insert a column for the ***Base*** instruction of the block in the ***Text Instructions Editor***.
2	In the ***Instruction box*** of the ***Text Instructions*** editor, select ***Flow*** and select the ***Linear Flow*** option as shown in the illustration below:



Note: If the column is changed, you will be asked if the linear flow rate or the default flow rate should be used. If the linear flow rate cannot be used due to the max flow rate of the system or new column, you will be advised that the max flow rate will be used instead.

6.6.7 Gradients and eluent concentrations

Introduction

Gradient instructions are given in the ***Text Instructions*** editor of the ***Method Editor***. This type of instruction defines gradients and immediate changes in eluent concentration.

Parameters of the Gradient

The table below shows the two parameters of the ***Gradient*** instruction:

Parameter	Description
Target	Final eluent composition expressed in % eluent B.
Length	Duration of the gradient.

Note: ***Mode A1/B1*** will utilize inlet valve position ***A1***. Mode ***A2/B2*** will utilize inlet valve position ***A2***. The inlet valve position cannot be changed if the ***%B*** value is greater than 0.

Example of a Gradient instruction

The starting point for the ***Gradient*** is always the current eluent composition. The instruction can be read as follows: "form a ***Gradient*** to reach ***Target*** after ***Length***".

Example of instruction

```
10.00 Gradient 50{%B}, 20{base}
```

The example instruction above forms a gradient to 50%B (***Target***) starting at breakpoint 10 with duration 20 method base units (***Length***). The example instruction will finish at breakpoint 30. If the current eluent concentration is greater than 50%, the gradient will be negative.

How to form a step gradient instruction

A step gradient is an immediate change in eluent composition. To form a step gradient, set the ***Length*** parameter to 0 in the ***Gradient*** instruction.

Example of instruction

```
10.00 Gradient 50{%B}, 0{base}
```

The example instruction above forms a step from the current eluent composition to 50%B at breakpoint 10. The method continues with 50%B.

Breakpoints for gradients

The breakpoint for a ***Gradient*** instruction defines the time or volume (according to method base) for the start of the gradient. A gradient with a non-zero duration occupies time and volume in the method, and breakpoints for other instructions may be set to occur before the gradient is completed. For most instructions, the instruction is simply carried out at the requested breakpoint, while the gradient is forming.

Instructions that affect gradients

The table below describes the instructions that affect the gradient:

Instruction	Effect
Gradient	A new gradient will start at the requested breakpoint. Any remaining duration of the previous gradient is ignored.
Flow	The eluent flow rate will change at the requested breakpoint. If the current base is volume or column volume, the duration of the gradient will be changed. If the method base is time, the volume of the gradient will be changed.
End_Method	The whole method will stop, interrupting the gradient.
End_Block	The gradient formation will continue uninterrupted unless a new ***Gradient*** instruction is issued in the next block. For example, this means that a block can be called conditionally during gradient formation without interrupting the gradient.

Gradients with variable length

For many purposes, it can be useful to define the length of the gradient as a variable. When this is done, breakpoints for instructions issued during or after the gradient in the same block are automatically shifted in proportion to the length of the gradient, with the same functionality as ***Change*** in the ***Text Instructions*** editor.

Instruction after a gradient

Any instruction that you want to insert after a gradient should be placed after the combined breakpoint and gradient length, since gradients function over time.

6.7 Standard Watch conditions

Introduction

Watch instructions allow the progress of a method run to be determined by the events during the method run, for example, start collecting fractions when the first peak eluates, or equilibrate the column until the eluent conductivity has reached a given value. This is facilitated by the ***Watch*** instructions.

The system strategy includes ***Watch*** instructions for each monitor defined in the system. These instructions are used to survey method runs, and instruct the system to call a specified block or an instruction when a particular monitor signal meets a given condition. As long as the condition is not met, the block is not activated.

Note: ***Watch*** instructions are shown in the ***Instruction box*** of the ***Text Instructions*** editor, indicated in the ***Block*** pane by a green line that shows the start and duration of the watch.

When is a Watch active?

The breakpoint when the ***Watch*** instruction is issued determines when the watch begins, not when the block is activated.

A watch is active from the point at which it is issued until

- the ***Watch*** condition is met

  or

- a new watch is set for the same monitor

  or

- a ***Watch_Off*** instruction is issued for the monitor.

How to insert a Watch instruction

Watch instructions are inserted in the ***Instruction box*** of the ***Text Instructions Editor***. The table below describes how to do this.

Step	Action
1	In the ***Breakpoint*** field, select the appropriate breakpoint. This decides when the watch begins.

Step	Action
2	• Select ***Watch*** in the ***Instructions*** field. • Select a ***Watch instruction*** from the list. • Select appropriate values under ***Test***, ***Value*** and ***Action*** in the ***Parameters*** field.
3	Click the ***Insert*** button. *Result:* The new ***Watch*** instruction is inserted on the list of actions in the ***Text*** window.

Test options in the Parameters field

The table below describes the ***Watch*** options that are available on the ***Test*** drop-down list of the ***Parameters*** field:

Option	Explanation
Greater_Than	The signal exceeds a certain value.
Less_Than	The signal falls below a specified value.
Slope_Greater_Than	The rate of change of the signal exceeds a specified value, expressed in monitor units/minute (for example, mAU/min).
Slope_Less_Than	The rate of change of the signal falls below a specified value, expressed in monitor units/minute (for example, mAU/min).
Less_Than_Or_Valley	The signal falls below a specified value or a valley is detected. A valley is detected only after a ***Peak_Max*** has been detected, and the valley is defined by a local minimum followed by an increase to 102% of the local minimum value plus the ***Delta_Peak*** value (see below).
Peak_Max	The signal falls to a specified fraction of the most recent peak maximum minus the ***Delta_Peak*** value. Factor=1 detects peak maximum.
Stable_Baseline	The signal is stable within the limits of the ***Delta_Base*** value for the period specified by the minutes parameter.

Note: For slope values, use the ***Differentiate*** function in the ***Evaluation*** module to measure the slope of the test chromatogram. The ***Simulate Peak Fractionation*** technique can also be used to find the slope values.

Watch conditions for air sensors and AuxIn

Two ***Watch*** conditions are available for systems with air sensors, although they may be handled differently depending on the system. The table below describes the conditions and their explanations:

Condition	Explanation
Equal 0	No air detected.
Equal 1	Air detected.

Note: To use the ***Watch_AirSensor*** instruction for air sensors, the ***Alarm_AirSensor*** setting must be disabled.

Actions when a Watch condition is met

The table below describes possible actions when a watch condition is met:

Instruction	Effect
Block name	Calls the named block.
Pause, ***Hold***	Pauses or holds the method.
Continue	Continues the method if paused or held.
End_block	Ends the current block and return to the point from which the block was called.
End_method	Ends the method.
Ready	Indicates that the next step in a ***MethodQueue*** may start.

How to enter settings for Delta_Peak and Delta_Base

Permanent settings

Permanent settings for ***Delta_Peak*** and ***Delta_Base*** are entered with the ***WatchPar*** instruction (for example ***WatchPar_UV***, ***WatchPar_Cond***) under ***System:Settings*** in the ***System Control*** module (see the Administration and Technical Manual).

Temporary settings that apply only for the duration of a given run can be entered in the Instructions field of the ***Instruction box*** in the ***Text Instructions*** editor. Select ***Alarms&Mon*** and then ***WatchPar***.

The Delta_Peak setting

The ***Delta_Peak*** setting helps the software to detect valleys, peaks and peak maximum, and to ignore noise in the chromatogram.

The ***Delta_Peak*** value should be set

- large enough so that signal noise does not activate the conditions

  and

- small enough so that the condition is activated close to the valley or peak.

As a general guideline, set the value to 2-3 times the noise level and 5-10% of the smallest expected peak height. If you set a too high value you can prevent a new peak from being detected after a local minimum.

Use of the Delta_Peak setting

The ***Delta_Peak*** setting

- sets the threshold for signal increase after a local minimum that will be interpreted as a valley for the ***Less_Than_Or_Valley*** condition. A valley and a new peak are detected when the signal increases to 102% of the local minimum plus the ***Delta_Peak*** value.

  Note: A valley is detected only after a ***Peak_Max*** has been detected.

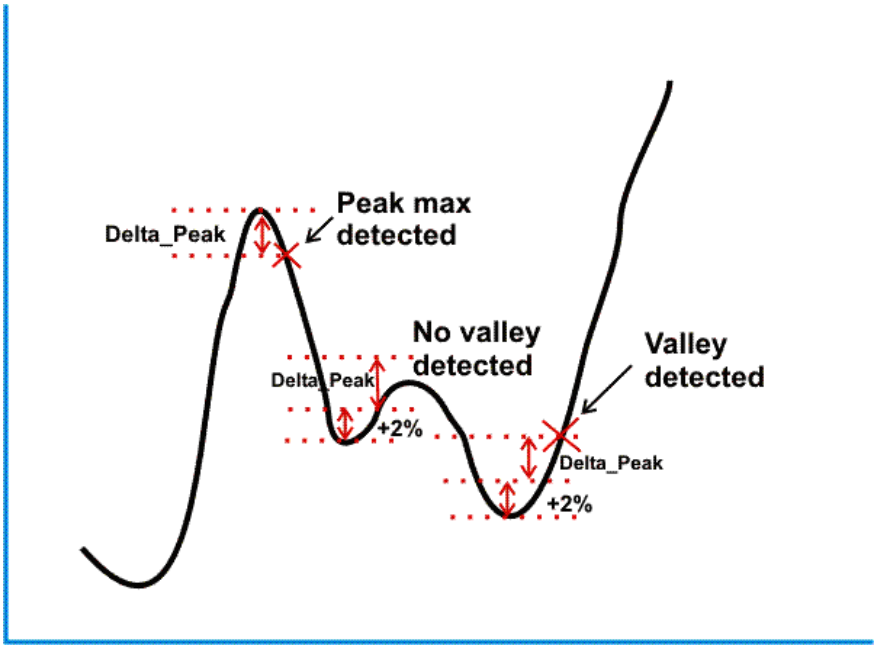
  Example:

  If there is a local minimum at 0.05 AU and a ***Delta_Peak*** of 0.01 AU, a valley will be detected at:

  `(1.02 x 0.05)+0.01=0.111 AU`

- sets the threshold for signal decrease after a local maximum that will activate the ***Peak_Max*** condition. ***Peak_Max*** is detected when the signal falls to the specified fraction of the most recent peak maximum minus the ***Delta_Peak*** value.

  The figure below illustrates the ***Delta_Peak*** setting where ***Peak_Max*** is detected when the signal falls by ***Delta_Peak*** from a local maximum if the ***Peak_Max factor*** is set to 1:



The Delta_Base setting

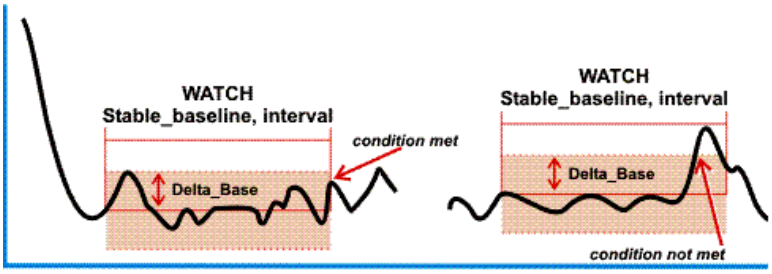
The ***Delta_Base*** setting helps the software to determine when the baseline is considered to be stable. In other words, it defines the permitted variation for the ***Stable_Baseline*** condition. For this condition to be activated, the signal may not vary by more than the ***Delta_Base*** value up or down over the time interval specified in the ***Stable_Baseline*** condition in the ***Watch*** instruction.

Note: The ***Delta_Base*** setting affects the ***Stable_Baseline*** condition only.

The condition Watch Stable_Baseline

The condition ***Watch Stable_Baseline*** is met if the signal does not deviate by more than ***±Delta_Base*** from the baseline during the time interval specified for the watch. The baseline value is determined by the signal at the start of the watch. If the condition is not met, a new interval is started with a new baseline value defined by the signal level at the start of the new interval.

The illustration below shows an example of this:


WATCH
Stable_baseline, interval
Delta_Base
condition met
WATCH
Stable_baseline, interval
Delta_Base
condition not met

6.8 How to save or delete a method template

How to save a method as a template

You can save a method that you have created yourself as a template if you have ***Edit global lists*** authorization (see the Administration and Technical Manual).

Recommendation

The templates for each system are common for all users. Be restrictive in saving methods as templates. We recommend that only methods that are useful for all users be saved as templates.

The table below describes how to save a method as a template:

Step	Action
1	Choose ***File:Save as Template*** in the ***Method Editor***. *Result:* The ***Save as Template*** dialog box is displayed.
2	Enter a name for the template in the ***Name*** field, *or* choose an existing template name from the ***Templates*** list that shows the available templates within the chosen system.
3	• Select the system for which the template is intended in the ***For system*** field. • Select the appropriate technique on the ***Technique*** list. • Select ***Any*** on the ***Technique*** list. • Click ***OK***. *Result:* The method is saved as a template.

How to delete a template

The table below describes how to delete a template:

Step	Action
1	Choose ***Edit:Delete template*** in the ***Method Editor***.

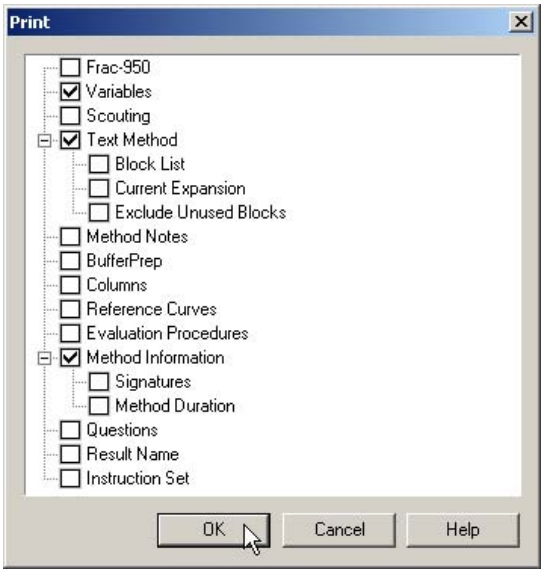
Step	Action
2	• Select the system and the template that you want to delete. • Click the ***OK*** button and the ***Yes*** button to confirm.

6.9 How to print a method

Instruction

You can print a copy of the method, including items from the method documentation, in ***Run Setup*** and the ***Text Instructions*** editor.

The table below describes how to print a method:

Step	Action
1	In the ***Method Editor***, select ***File:Print*** *or* click the print icon. *Result:* The ***Print*** dialog box is displayed, showing the available items from the ***Method Editor***. 

Step	Action
2	• Select the options you want to print. • Click ***OK***. *Note:* For comments on the different alternatives, see "The Print dialog box" below.

The Print dialog box

The table below describes some of the check box options in the ***Print*** dialog box:

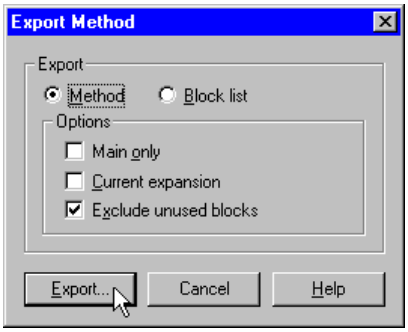
Check box	If you select this box...
Text Method	all instructions will be printed, including those in unused blocks.
Text Method:Current Expansion	the method will be printed according to the current expansion in the ***Text*** pane. (Only available from the ***Text Instructions*** editor.)
Exclude Unused Blocks	only blocks that are used in the method will be printed.
Text Method: Block List	only the main method and a list of the blocks that are used in the method will be printed.

6.10 How to export a method

Instruction

You can easily export a method to another file, and save it in another format, for instance .rtf. This is useful when you want to enable others to read the methods without having access to UNICORN on their computers.

The table below describes how to export a method and save it to another file:

Step	Action
1	In the ***Text Instructions*** editor or the ***Run Setup***, select ***File:Export:Method***. *Result:* The ***Export Method*** dialog box is displayed. 
2	Do the following: • Select whether the current method should be exported as a ***Method*** or as a ***Block list***. • Select the appropriate boxes in the ***Options*** field to define the level of detail in the information. • Click the ***Export*** button. *Result:* The ***Export Method to file*** dialog box is displayed.
3	• Enter a file name and select the target drive and folder. • Click the ***Save*** button.

7 Scouting

Introduction

Scouting is used to repeat a series of ***Method runs*** automatically with predetermined changes in the values for one or more ***Variables***. A ***Scouting Scheme*** is defined as part of the method.

This chapter describes how to set up a ***Scouting Scheme*** and define columns. The chapter also provides some usage examples.

In this chapter

This chapter contains these topics:

Section	See page
7.1 How to set up a Scouting Scheme	214
7.2 How to define different columns for scouting	220

7.1 How to set up a Scouting Scheme

Introduction

This section describes how to set up a method for scouting.

Any parameter can be scouted, provided that it can be defined as a variable in the method.

Note: Scouting schemes can only be set up for ÄKTAxpress systems when the UNICORN software has been installed in classic mode.

When to use scouting

Scouting is a facility for automatically repeating a run with systematic variation of one or more parameters. Some typical situations where scouting is useful are when you want:

- to screen for the best column
- to find the optimal pH
- to test column capacity (sample volume)
- to find the optimal flow rate for binding and elution
- to optimize gradient length and slope
- to optimize step gradients.

Variable values

The variables that appear in the scouting scheme are usually a subset of those on the ***Variables*** tab of the ***Run Setup***. The values in the scouting scheme can only be set on the ***Scouting*** tab, while the default values in the method can be set either on the ***Variables*** tab or in the ***Text instruction*** pane.

Changing variable values in the scouting scheme does *not* change the values on the ***Variables*** tab or in the text instructions. Values for variables selected for scouting are grey on the ***Variables*** tab and cannot be changed there.

Any changes that you make to variable values when a scouting scheme is run are saved in the result file. Results from a scouting run are saved in a scouting folder.

Scouting tab buttons

There are seven buttons on the ***Scouting*** tab of the ***Run Setup*** plus the ***Help*** button. The table describes the functions of these buttons:

Click the button...	if you want...
Define...	to define new scouting variables. The ***Scouting Variables*** dialog box is displayed, and you can select variables to be used in the scouting series. *Note:* The variables that have been selected for scouting *cannot* be changed on the ***Variables*** tab.
Clear All	to clear all runs. This converts the scouting run to a non-scouting run so that it contains only the original method and values.
Delete	to remove a run from the ***Scouting*** tab. Click on any variable in the run you want to remove, and then click the ***Delete*** button.
Insert	to insert a new scouting run before an existing run. Click on a run column and then click the ***Insert*** button. The new run will inherit the variable values from • the preceding run, *or* • from the default values in the method if the run is inserted at the beginning of the scouting series
Add	• to add a scouting run if there are no runs previously in the scheme. Default values will be used for the first run. *or* • to add a scouting run after all other runs in the series. The new run inherits the values from the run that precedes the new run.
Series...	to set up a series of runs with differing inputs.
Edit Variable...	to rename or delete a variable, or change a variable into a detail variable.

How to set up or edit a Scouting Scheme

The table below describes how to set up or edit a scouting scheme.

Step	Action
1	Create a method. If you do not use a template or wizard, define appropriate variables in the method.
2	In the ***Run Setup***, click the ***Scouting*** tab. *Result:* If no scouting variables have been previously defined, the ***Scouting Variables*** dialog box is displayed. If not, click the ***Define*** button.
3	Select the variables you want to scout. If you cannot find the variable you want, use the following options: • ***Show details*** to display variables created with the ***Visible in details only*** option. • ***Show unused variables*** to display all variables, including those that are not used in the method. Click ***OK***. *Result:* The selected scouting variables will appear in a column, with default valued inserted.
4	Make any required changes in the scouting variable values.
5	To add a new ***Run*** column, click the ***Add*** button to copy the values from the last run column, and then change variable values as required.
6	Repeat steps 3 to 5 as required until you have defined all the scouting runs you need.
7	To exclude scouting runs from the default scouting scheme, right-click the heading of the run. To include the scouting run again, right-click it again.

Step	Action
8	Click the ***Start Protocol*** tab in ***Run Setup***. **Select from the following options:** • The ***Scouting*** box: Select this to display the ***Scouting*** page at the start of a run. This allows the operator to adjust the values for scouting variables before the method run starts. • The ***First run only*** button: Select this to display the start protocol before the first run only. The settings entered in the ***Start Protocol*** for the first run will apply throughout the run, and the scouting series will be performed automatically without user intervention. • The ***All runs*** button: Select this to display the ***Start Protocol*** before each run in the scheme. This gives the operator an opportunity to change variable values or fill the sample loop before each run. *Note:* The operator must then click the ***Start*** button before each run.

How to set up series

The table below describes how to set up series.

Step	Action
1	Select a cell on the ***Scouting*** tab, and click the ***Series*** button. *Result:* The ***Insert Series*** dialog box is displayed.
2	In the ***Insert Series*** dialog box, type the selected series values (within the specified range limits), separated by commas, and click OK. *Result:* A new set of runs is inserted on the ***Scouting*** tab with the values provided.

How to delete or rename scouting variables

Scouting variables can be deleted or renamed in the scouting scheme in the same way as in the ***Variables*** tab. The table below describes how to delete or rename a variable in the ***Scouting*** tab.

Step	Action
1	Click the ***Edit Variable...*** button on the ***Scouting*** tab. *Result*: The ***Edit Variables*** dialog box opens. The variables are listed alphabetically.
2	Select the variable to edit.
3	**Rename** • Type a new variable name in the ***New name*** text box. • Click the ***Rename*** button. *Result*: The variable is renamed. **Delete** • Click the ***Delete*** button. • Confirm that you want to delete the variable. *Result*: The variable is deleted.

How to change a scouting variable into a detail variable

Detail variables are indicated with a ***D*** to the left of the ***Variable*** column on the ***Scouting*** tab. The table below describes how to set up a detail variable.

Step	Action
1	Click the ***Edit Variable...*** button on the ***Scouting*** tab. *Result*: The ***Edit Variables*** dialog box opens. The variables are listed alphabetically.
2	Choose the variable to be changed.

Step	Action
3	• Select the ***Set visible in details only*** checkbox. • Click the ***Close*** button. *Result*: The variable is indicated by a ***D***. *Note*: De-select the checkbox to make the variable fully visible again.

How to copy contents to factorial design programs

The contents of the ***Scouting*** tab can be copied and pasted into a third-party factorial design program. Processed values can then be pasted back into the ***Scouting*** tab. The table below describes how to do this:

Step	Action
1	Select the text, etc., that you want to copy.
2	Press ***Ctrl+C***.
3	Place the cursor where you want to insert the copied text.
4	Press Ctrl+V.

7.2 How to define different columns for scouting

Instruction

You can define different columns for use in the various scouting runs. However, in selecting a different column, other variables may also be changed between runs. The table describes how to scout columns.

Note: Scouting can only be performed on ÄKTAxpress systems when the UNICORN software has been installed in classic mode.

Step	Action
1	Choose a method with a column (not ***Any***). Alternatively, you can have a method with CV as the main base and a column (not ***Any***) selected as a variable called "column".
2	Click the ***Define*** button on the ***Scouting*** tab. *Result:* The ***Scouting Variables*** dialog box is displayed.
3	Select ***Column*** and click ***OK***.
4	Click the ***Column*** drop-down menu item within the desired run. *Result:* A menu is displayed.
5	Select a column. *Result:* The ***Column Value Update*** dialog box is displayed.
6	The dialog box asks you whether you want to update the instructions with column default values. Select one of the following: ***Yes*** The method for the scouting run is updated with variable parameter values for the selected column, consisting of UV average time, pressure limit, flow rate, etc. These parameter values are added to the scouting variables on the ***Scouting*** tab. Note that the updated parameter values may differ from the values for the same variables in other scouting runs. ***No*** No changes are made. The method retains the parameter values corresponding to the column that were either originally selected during creation of the method, or included in an earlier version of the method on the ***Scouting*** tab for which the default values for that column were accepted. *Note*: If the method contains a linear flow rate instruction, the user can keep the linear flow rate by selecting a check box in the dialog box.

8 MethodQueues

Introduction

MethodQueues provide a means for linking several methods together, on the same or different systems. For example, if a system wash procedure is programmed in a separate method, it can be linked in a ***MethodQueue*** to a series of different process methods, ensuring that the same wash procedure is used before every process. Alternatively, the product of a separation on one system might form the starting material for a separation on the next, allowing fully automated multi-step processing.

MethodQueues are used to set up a number of runs in series. For example:

- ***Synthesis No. 1*** in column 1
- ***Synthesis No. 2*** in column 2
- ***DEA treatment*** for ***Synthesis No. 1*** in column 1
- ***DEA treatment*** for ***Synthesis No. 2*** in column 2

In this chapter

This chapter contains these topics:

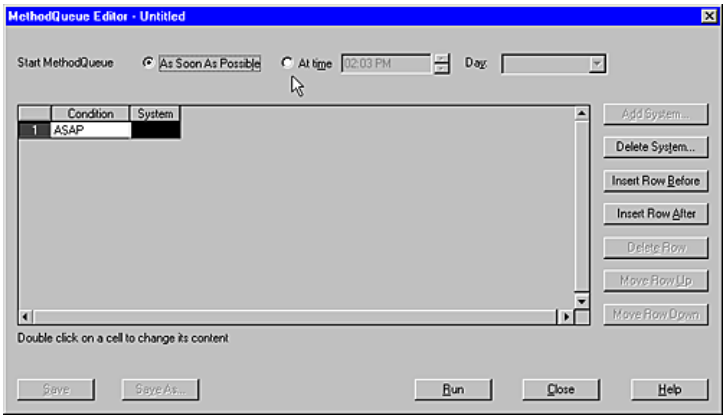
Section	See page
8.1 How to create a new MethodQueue	222
8.2 How to edit a MethodQueue	227

8.1 How to create a new MethodQueue

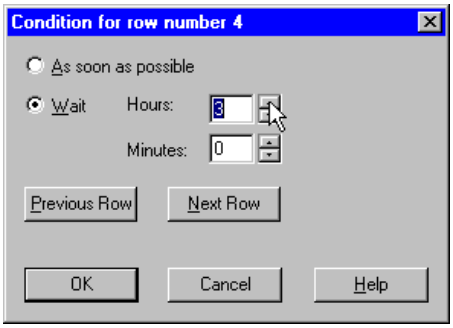
Instruction

The table below describes how to create a ***MethodQueue*** in the ***UNICORN Manager*** module.

Note: You can only create a ***MethodQueue*** for ÄKTAxpress systems if the UNICORN software has been installed in classic mode.

Step	Action
1	• Select ***File:New:MethodQueue***. *or* • Right-click in the ***Methods*** window and select ***New:MethodQueue*** on the shortcut menu. *or* • Click the ***MethodQueue*** icon. *Result:* The ***MethodQueue Editor*** dialog box is displayed. 
2	The default selection for ***Start MethodQueue*** is ***As soon as possible***. • Click the ***At time*** radio button and select a time and weekday for the start of the ***MethodQueue***, if desired.

Step	Action
3	• Double-click the cell in the first row of the ***System*** column. *Result:* The ***Method for row number 1 System*** dialog box opens. *Note*: See "How to set up MethodQueues on several systems" below if you have more than one system available.
4	• Select a method and click ***OK***. *Result:* The method is displayed in the ***System*** column.

Step	Action
5	• Click the ***Insert Row After*** button and repeat steps 3 and 4 to add more methods to the ***MethodQueue***. *Note:* The timing of ***MethodQueue*** steps performed on different systems can also be controlled by the ***Ready*** instruction in the method (see "Relative timing of steps" below). By default, each method step will start as soon as possible (***ASAP***) after the completion of the previous method step. Use the ***Condition*** cell of the chosen method to set another time interval for starting a selected step. • In the ***Conditions*** column, double-click the cell for the method to be delayed. *Result*: The ***Condition for row number X*** dialog box opens.  *Note*: Use the ***Previous Row*** and ***Next Row*** buttons to select other methods for editing. • Click the ***Wait*** radio button, select the number of hours and minutes that the method is to be delayed and click ***OK***. *Result*: The execution of the ***MethodQueue*** will be held for the selected number of hours and minutes and then resume. • Click the ***Save*** button to save the method. Result: The ***Save MethodQueue*** dialog box opens. • Type a file name and click the ***Save*** button.

How to set up MethodQueues on several systems

If you have more than one system available, the ***System*** column will not be displayed at first in the ***MethodQueue Editor***. The table below describes how to set up a ***MethodQueue*** for several systems.

Step	Action
1	• Click the ***MethodQueue*** icon. • Click the ***Add System*** button and select a system for the first ***MethodQueue*** step from the ***Add System*** dialog box.
2	• Repeat this for each system when you want to use a different system in the ***MethodQueue***. *Result*: Another system column will be added for each additional system.

Relative timing of steps

The setting of the ***Condition*** dialog box (reached by double-clicking a ***Condition*** cell in the ***MethodQueue Editor*** dialog box), determines the relative timing of the steps of a ***MethodQueue***. If successive methods are run on the same system, the timing set in ***Condition*** applies from the completion of one method to the start of the next.

If successive methods are run on different systems, you can use the ***Ready*** instruction in one method to trigger the start of the next method. In this way, you will be able to start the next method before the current method has ended. The ***Condition*** setting then applies from the ***Ready*** instruction to the start of the triggered method. This is useful in situations where a method on one system prepares the starting material for the next, and then continues to wash the system. See the example below:

Instruction to System 1	Instruction to System 2
Apply sample	
Eluate	
READY	***Apply sample***
Wash	***Eluate***

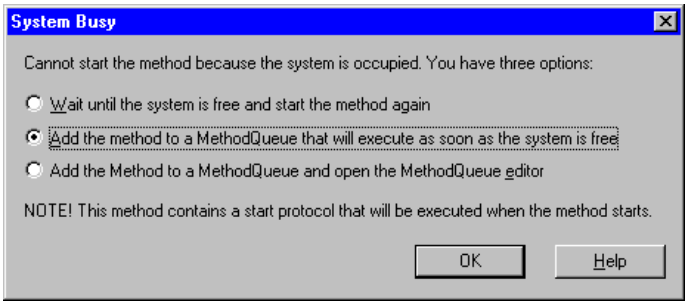
Unattended operation of the MethodQueue

The ***Start Protocol*** for each method step in the ***MethodQueue*** is displayed when the corresponding method is run. If you want the ***MethodQueue*** to operate unattended you must ensure that the methods do not include a ***Start Protocol***.

See *Chapter 5 How to create a method, on page 97* for more information.

How to hold a method in queue while the system is busy

The table below describes how you can create a ***MethodQueue*** if you try to start a new method run while the system is still busy with another method run.

Step	Action
1	Right-click on the method in the ***UNICORN Manager*** module and select ***Run:****system name* on the shortcut menu. *Result*: The ***System Busy*** dialog box opens. 
2	• Select the ***Add the method to a MethodQueue that will execute as soon as the system is free*** option. • Click ***OK***. *Result*: A ***MethodQueue*** will automatically be created in the default queue folder. The name of the ***MethodQueue*** will be the same as the method name, followed by a five-digit sequence number.
3	The method will be executed as soon as the system is free. *Note*: A warning note is displayed in the ***System Busy*** dialog box if the method includes a ***Start Protocol***. The ***Start Protocol*** must be completed at the start of the method run before it can be executed.

8.2 How to edit a MethodQueue

Method Queues are saved in a separate folder

MethodQueues are saved in a separate folder within the folder that you specified when you saved the ***MethodQueue***. The ***MethodQueue*** folder is represented by a special icon in the ***Methods*** window of the ***UNICORN Manager***.

A ***MethodQueue*** folder contains the ***MethodQueue*** definition and copies of all included methods.

How to edit a MethodQueue file

The ***MethodQueue*** files are *copies* of the original method files. If changes are made in the original method, these will not affect the method in the ***MethodQueue***.

To avoid confusion between different versions of method files, make sure that ***MethodQueue*** definitions always contain updated methods. To implement changes in a ***MethodQueue*** method, do one of the following:

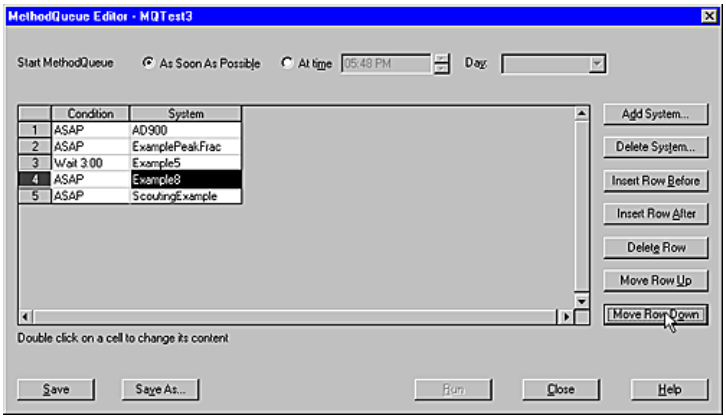
- Edit the method in the ***MethodQueue*** folder,

  or

- Edit the original method, then use the ***MethodQueue*** editor to update the ***MethodQueue***, and replace the old method with the changed version.

Instruction

The table below describes how to edit an existing ***MethodQueue***.

Step	Action
1	Right-click the selected ***MethodQueue*** folder icon in the ***UNICORN Manager***, and select ***Edit*** from the displayed menu. *Result:* The ***MethodQueue Editor*** dialog box is displayed. 
2	Select a table row to edit and do the following as required: • Double-click the ***System*** cell and select a new method from the ***Method for row...*** dialog box. • Double-click the ***Condition*** cell and edit the delay time for the method. • Click the ***Add System*** button to add a new system to the queue and use it for a ***MethodQueue*** step. • Click the ***Delete System*** button to remove a system and all associated methods from the ***MethodQueue***. • Click the ***Insert Row Before*** or ***Insert Row After*** buttons to add new rows before or after the selected row. • Click the ***Delete Row*** button to remove the selected row. • Click the ***Move Row Up*** or ***Move Row Down*** to move the selected row one step up or down in the queue.
3	• Click the ***Save*** button. • Click the ***Run*** button to execute the ***MethodQueue*** immediately or the ***Close*** button to close the dialog box.

9 How to perform method runs

Introduction

This chapter describes how to perform and monitor different kinds of method runs from the ***System Control*** module. It also describes how to control the system with manual commands and instructions.

In this chapter

The chapter contains these sections:

Section	See page
9.1 How to start a method run	230
9.2 How to monitor a method run	234
9.3 Manual system control	251
9.4 How to perform a scouting run	260
9.5 How to perform a MethodQueue run	262
9.6 If the network connection fails	265

9.1 How to start a method run

Before you start

Before you start a method, make sure that

- the correct system is connected in control mode
- the correct system for the method is selected in the system selector of the ***System Control*** module
- the system is prepared according to the system user manual

Note: If the system is connected via a ***CU-950 Advanced*** unit, the Ethernet connection must not be broken during the start-up phase of the method run.

How to start from the UNICORN Manager

You can start a method from the ***UNICORN Manager*** in two ways:

- Select a method in the ***Methods*** window and select ***File:Run***.
- Select a method, right-click and select ***Run*** from the displayed menu.

How to start from System Control

The table below describes how to start a method run from ***System Control***:

Step	Action
1	• Select ***File:Run*** or • click the ***Run*** button. *Result:* The ***Run*** dialog box is displayed. **Note:** The ***Run*** button will open the method that was used for the previous run, if a run has been performed since you logged on.
2	Select a method and double-click the method icon. *Result*: The method run starts. If the method includes a ***Start Protocol*** this must be completed before the actual method run starts. See further instructions below.

How to add methods to the File menu

For methods that are used frequently (for example column cleaning methods or routine separations), it may be convenient to define the methods as commands in the ***File*** menu.

The table below describes how to define a method as a command:

Step	Action
1	Choose ***File:Menu*** in ***System Control*** and select the required method.
2	Click the ***Add*** button and click ***OK***. *Result:* The method name will appear as a command in the ***File*** menu. If you choose the command, the method will start.

How to start an instant run

You can start a method template or wizard directly if your system has defined templates or wizards.

To do this, either

- click the ***Instant Run*** icon in the ***UNICORN Manager*** toolbar

or

- select ***File:Instant Run*** in ***System Control***.

How to use the Start Protocol

If the method is defined with a ***Start Protocol***, this will be displayed before the method actually starts.

The table below describes how to use the ***Start Protocol***:

Step	Action
1	• Start the method run. • Work through the start protocol, answering questions as required. The start protocol items that can be displayed are described in *Section 6.5.14 The Start Protocol tab, on page 185*. • As each screen is completed, click the ***Next*** button to move to the next screen or the ***Back*** button to return to the previous screen.
2	Click the ***Start*** button in the last window to start the run.

Confirm/Sign authorization for the Start Protocol

If there are any questions in the ***Start Protocol*** that require authorized confirmation, you will be asked for a user name and password when you attempt to leave the screen containing the questions. Only users with ***Confirm/Sign*** authorization may authorize answers to such questions. Each question that requires an authorization must have a separate authorization.

How to start a method when the system is busy

If the system is busy with a method run in progress, you can still start a new method. You will have the option to place the method in a ***MethodQueue***, which can be executed as soon as the system becomes available again. The table below describes how to do this.

Note: MethodQueues are only available for ÄKTAxpress systems if the UNICORN software has been installed in classic mode.

Step	Action
1	• While a method run is in progress, right-click on the next method you want to run and select ***Run:System***. *Result*: The ***System Busy*** dialog box opens.
2	• Select the ***Add the method to a MethodQueue that will execute as soon as the system is free*** option. • Click ***OK***. *Result*: A ***MethodQueue*** will automatically be created in the default queue folder. The name of the ***MethodQueue*** will be the same as the method name, followed by a five-digit sequence number.

Step	Action
3	The method will be executed as soon as the system is free. **Note:** A warning note is displayed in the ***System Busy*** dialog box if the method includes a ***Start Protocol***. The ***Start Protocol*** must be completed at the start of the method run before it can be executed.

Note: See *Section 8.2 How to edit a MethodQueue, on page 227* for more information.

9.2 How to monitor a method run

Introduction

This section describes how to monitor a method run by using the ***System Control*** module and how to customize the different panes.

In this section

The table shows the topics that can be found in this section.

Section	See page
9.2.1 How to customize System Control panes	235
9.2.2 The Run Data pane	237
9.2.3 The Curves pane	240
9.2.4 The Flow Scheme pane	247
9.2.5 The Logbook pane	249

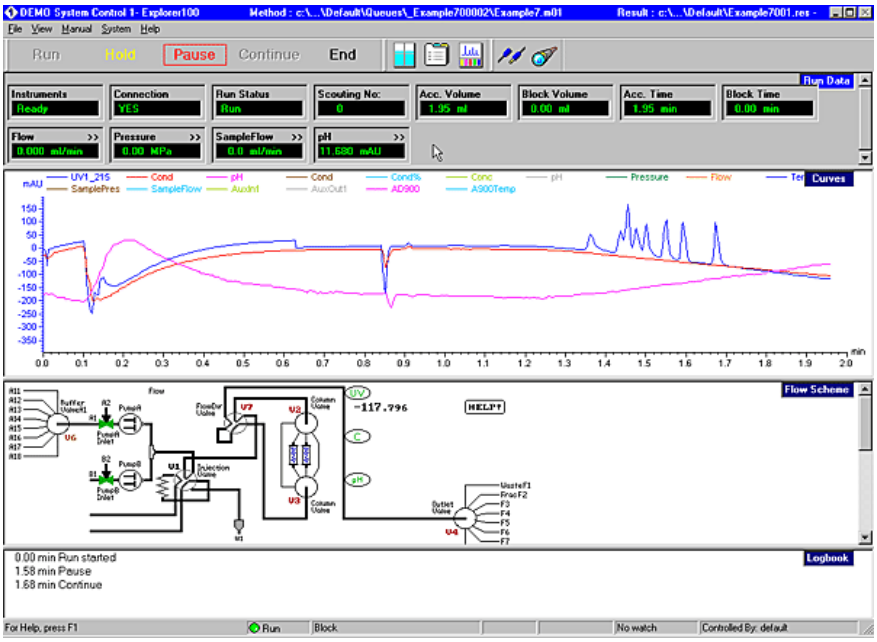
9.2.1 How to customize System Control panes

Introduction

The ***System Control*** module displays the status of the current system. On the Windows taskbar, there may be up to four ***System Control*** modules available that can be connected to different systems. Separate systems may be controlled and displayed independently of each other.

Illustration

The illustration shows the ***System Control*** module with the ***Run Data***, ***Curves***, ***Flow scheme*** and ***Logbook*** panes displayed.



How to select what panes to display

Each ***System Control*** module displays up to four panes for monitoring different aspects of the run. To select what panes to display, either

- click the ***Customize Panes*** icon,

or

- choose ***View:Panes***.

How to customize System Control panes

Change the size

Select a split-bar and drag up and down to change the size of a specific pane.

Maximize, restore or hide

Right-click a pane and select the appropriate option to:

- maximize,
- restore

or

- hide the pane.

9.2.2 The Run Data pane

Description

The ***Run Data*** pane displays the current values for selected run parameters. The update interval is defined in the system strategy.

The figure below displays an example of the ***Run Data*** pane:

How to change the appearance of the pane

The appearance of the pane can be changed so that it includes more or fewer data displays. The table below describes how this is done:

Step	Action
1	• In ***System Control***, select ***View:Properties*** *or* • right-click on the pane and select ***Properties*** on the menu. *Result:* The ***Properties*** dialog box is displayed.
2	Select the ***Run Data Groups*** tab and, if desirable, do one or more of the following: • *Select* an available group to be displayed in the list to the left. • *Edit* an available group: Select the group from the list on the left, and click the ***Edit Group*** button. Modify the included readings in the list to the right, and click ***OK***. • *Create* a new group: Click the ***New group*** button and select the readings that you want to view from the list. Enter a name for the group, and click ***OK***. • *Delete* a group: Click the ***Delete Group*** button and select a group in the ***Delete Layout*** dialog box, click ***OK*** and confirm the deletion.
3	Select the run data parameters that you want to display in the list to the right.

Step	Action
4	Click ***OK*** to view the selected items in the ***Run Data*** pane. The name of the selected layout replaces the default layout name ***Run Data***.

How to change text color or text background

The table describes how to change the text color or background in the displayed reading boxes.

Step	Action
1	Right-click on the pane and select Properties. *Result:* The ***Properties*** dialog box is displayed.
2	Select the ***Run Data Color*** tab.
3	Click the ***Text*** or ***Background buttons.*** Select a new color, and click ***OK***. *Result:* The color change is displayed in the test field.
4	Make further adjustments to the colors as appropriate.
5	Click ***OK*** to apply the changes.

How to set the pressure units

If the ***Pressure*** reading box is displayed in the ***Run Data*** pane, you can set the displayed units. The table below describes how this is done:

Step	Action
1	Right-click on the ***Pressure*** reading box to display the menu.
2	Select ***Set Unit*** and the appropriate unit (***MPa***, ***bar*** or ***psi***). *Result:* The selected unit is displayed.

How to view and select manual instructions

Some strategies directly link specific manual instructions to the reading boxes in the ***Run Data*** pane. This is indicated by a double arrow (**>>**). A particular reading box can have one or more instructions attached to it. In cases where there is more than one instruction, one of the instructions is the main instruction.

There are two ways to view the manual instructions:

Option 1:

- Double-click the reading box.

  Result: The dialog box for manual instructions is displayed, showing the instruction, or main instruction if there is more than one.

Option 2:

- Right-click the reading box. Select ***Instructions*** in the displayed menu. Another menu shows the specific manual instruction(s).
- Click an instruction to select it.

Result: The dialog box for manual instructions is displayed in which you can execute the appropriate command.

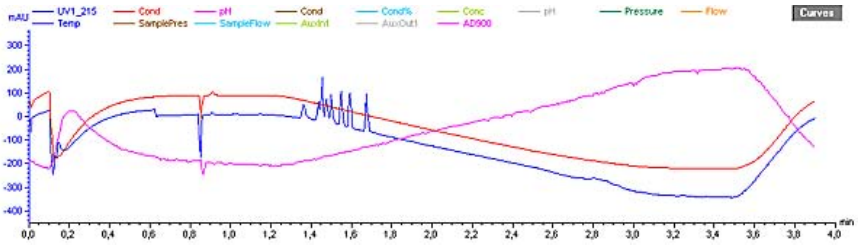
For more details on how to use manual instructions, please see *Section 9.3.2 Manual instructions, on page 256*.

9.2.3 The Curves pane

Introduction

The ***Curves*** pane of the ***System Control*** module displays monitor signal values graphically.

The figure below shows an example of the ***Curves*** pane:



How to select curves to be displayed

You can decide which curves you want to display in the ***Curves*** pane. Curves will only be shown for components present in the chromatography system.

The table describes how to select the curves to be displayed on the screen.

Step	Action
1	In ***System Control***, select ***View:Properties***. *Result*: The ***Properties*** dialog box is displayed.
2	Select the ***Curves*** tab. **Note:** The curves in the list are those for which ***Store*** is set to ***On*** in the system settings, together with any reference curves defined in the method.
3	In the ***Display curves*** list, select the curves you want to display. If you want all curves to be displayed, click the ***Select All*** button. If you do not want any curves to be displayed, click the ***Clear All*** button.
4	Click ***OK***.

How to display a vertical marker line

The table below describes how to display a vertical marker line:

Step	Action
1	Right-click the ***Curves*** pane and select ***Marker***.
2	Drag the marker line with the mouse. *Result:* Where the line bisects the curve, the X-axis and Y-axis values are displayed at the top right corner of the pane.

Note: Right-click and select ***Snapshot*** to record the marker position values. See *Section 2.2.7 Snapshots, on page 50* for more information about the ***Snapshot*** function.

How to set a reference point

When the vertical marker is displayed, you can set a reference point to display curve data. The table describes how to set a reference point:

Step	Action
1	• Display a ***Marker*** in the ***Curves*** pane. • Right-click and select ***Set Marker Ref. Point*** to define a reference point for the marker position.
2	When the marker is moved from the reference point, the X-axis and Y-axis values for the new position are displayed together with: • the new position in relation to the position of the reference point, • the minimum, maximum and average values for the curve interval between the reference point and the new position.

How to change the curve colors and styles

The ***Curves*** pane displays graphs for the selected curves in different colors, with any reference curves included with the method as dashed lines.

The table below describes how to change the curve colors and styles:

Step	Action
1	Select ***View:Properties***. *Result:* The ***Properties*** dialog box is displayed.
2	Select the ***Curve Style and Color*** tab.
3	• Select a curve from the ***Curve*** list. • Select an appropriate color and style.

How to change the scale of the Y-axis

In most cases, the Y-axis is automatically scaled for each of the curves. Values on the Y-axis apply to the curve with the same color as the axis markings. To get the correct Y-axis, click the legend. The table below describes how to fix the scale of individual curves.

Step	Action
1	• Select ***View:Properties***. *Result:* The ***Properties*** dialog box is displayed. • Select the ***Y-axis*** tab.
2	• Select the appropriate curve. • Select ***Fixed*** and type a minimum and maximum range in the fields within the specified limits.
3	Repeat step 2 for other curves if needed.
4	Click ***OK***.

How to change the scale of the X-axis

The table below describes how to change the scale of the X-axis:

Step	Action
1	• Select ***View:Properties***. *Result:* The ***Properties*** dialog box is displayed. • Select the ***X-axis*** tab.
2	Select the appropriate base, ***Time*** or ***Volume***. **Note:** Curves are collected in time and recalculated for display in volume. Thus, the resolution of the two bases may appear slightly different.
3	Select the appropriate ***Axis scale***: • ***Total*** will show the curves as far as they have come in the run. • ***Window*** allows you to set the portion of the total pane to be displayed, either in minutes or ml depending on the selected base. • ***Adjust retention zero to injection*** sets the retention value to zero at the point of the first injection. • Click ***OK***.

How to switch between time and volume units

- Click the legend of the X-axis

or

- right-click and select ***Base Type***

to switch the display between time and volume units. The run is controlled according to the time/volume base defined in the current block, regardless of the base in the curves display.

How to zoom in the Curves pane

The table below describes how to zoom in on a selected region of the curve pane:

Step	Action
1	• Press and hold the left mouse button and drag a rectangle out on the screen to encompass the area to be viewed. • Release the mouse button. *Result:* The display is now zoomed in on the selected area.
2	Repeat the process for further magnification of selected areas.

How to zoom out

To reduce the scale of the zoom, right-click in the ***Curves*** pane, and select one of the following options:

- ***Undo Zoom***: reverses each zoom-in action a step at a time.
- ***Reset Zoom***: reverses all zoom-in actions to the default scale.

How to select curve pressure units

If the ***Pressure*** curve is displayed in the ***Curves*** pane, you can set the displayed units. The table below describes how to do this:

Step	Action
1	Right-click in the ***Curves*** pane, and select ***Properties*** in the displayed menu. *Result:* The ***Properties*** dialog box is displayed.
2	Select the ***Y-Axis*** tab.
3	Select the ***Pressure*** curve and select the appropriate ***Pressure unit*** button. Click ***OK***.

How to edit text in the Curves pane

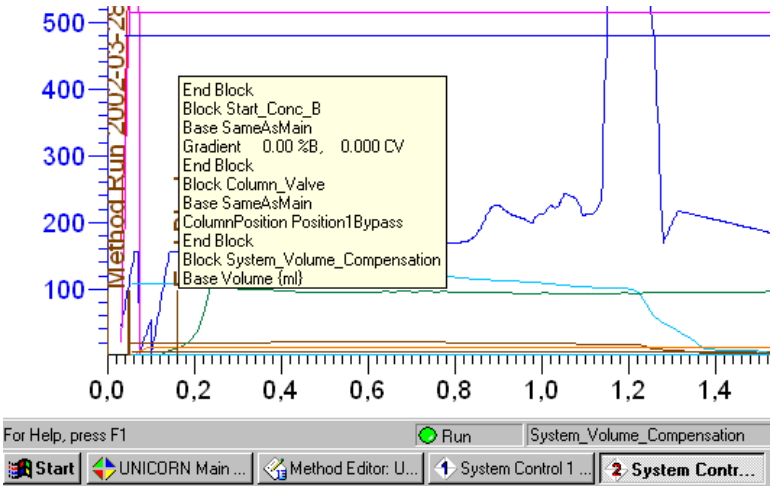
You can select the way that text is aligned for the ***Logbook*** and ***Fraction*** curves. You can also select to show only part of the ***Logbook*** information. The table below describes how to do this:

Step	Action
1	Right-click in the ***Curves*** pane, and select ***Properties*** in the displayed menu. *Result:* The ***Properties*** dialog box is displayed.
2	Select the ***Curve Style and Color*** tab.
3	Select the following: • ***Logbook*** or ***Fraction*** curve in the ***Curve*** list as appropriate. • Select the appropriate ***Logbook text alignment*** or ***Fraction text alignment*** option: - Horizontal - Vertical - Fly over (displays the text if you place the mouse pointer over the generated mark).
4	To filter the type of ***Logbook*** information overlaid on the ***Curves*** pane, do the following: • Click the ***Filter*** button. *Result:* The ***Filter Logbook*** dialog box is displayed. • Select the appropriate check boxes and set the maximum block depth. • Click ***OK*** to return to the ***Curve style and Color*** tab.
5	Click ***OK***.

How to view the complete logbook information

At some breakpoints there can be more logbook information than what is possible to conveniently display in the ***Curves*** pane. The additional information that is not displayed is indicated by an arrow point symbol by the break point.

- Hold the mouse cursor over the break point to display the complete information in a flyover text box, as shown in the illustration below.



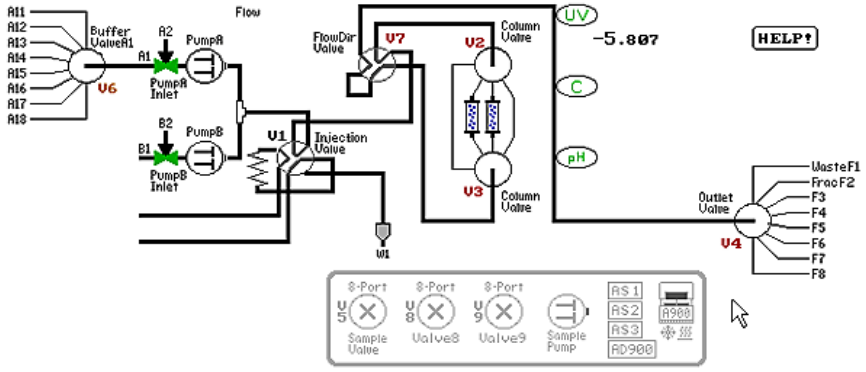
9.2.4 The Flow Scheme pane

Introduction

The flow scheme is a graphical representation of the chromatography system that shows the current status of the run. During a run, the flow scheme displays open flow path(s) in color and monitor signals with numerical displays.

Illustration

The illustration below shows an example of a flow scheme for a run:



How to stretch a flow scheme

The flow scheme can be stretched to fit the screen. To do this, right-click in the pane and select ***Stretch*** in the shortcut menu.

How to view and select flow scheme manual instructions

Some strategies link specific manual instructions directly to the components in the flow scheme pane. The components in the flow scheme that are associated with instructions are indicated with double arrows (**>>**). A particular component can have one or more instructions attached to it. In cases where there is more than one instruction, one of the instructions is the main instruction.

To display and select instructions:

- double-click a component

or

- right-click a component, select ***Instructions*** and an instruction in the shortcut menu.

Result: The manual instructions dialog box for the selected instruction type opens.

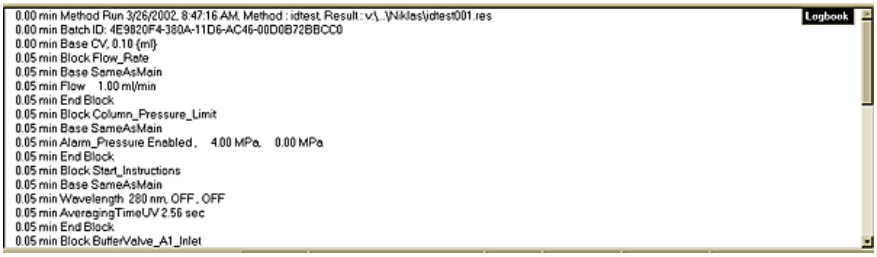
9.2.5 The Logbook pane

Introduction

All actions (including method start and end, base instruction, method instructions and manual interventions such as ***Pause*** or ***Hold***) and unexpected conditions such as warnings and alarms are logged for every run, with date, time and current user name where appropriate. The logbook thus provides a complete history of any given run. The log is saved in the result file.

Illustration

The illustration below shows an example of the ***Logbook*** pane:


Logbook
0.00 min Method Run 3/26/2002, 8:47:16 AM, Method : idtest, Result : v:\...\Niklas\idtest001.res
0.00 min Batch ID: 4E9820F4-380A-11D6-AC46-00D0B72BBCC0
0.00 min Base CV, 0.10 {ml}
0.05 min Block Flow_Rate
0.05 min Base SameAsMain
0.05 min Flow 1.00 ml/min
0.05 min End Block
0.05 min Block Column_Pressure_Limit
0.05 min Base SameAsMain
0.05 min Alarm_Pressure Enabled , 4.00 MPa, 0.00 MPa
0.05 min End Block
0.05 min Block Start_Instructions
0.05 min Base SameAsMain
0.05 min Wavelength 280 nm, OFF , OFF
0.05 min AveragingTimeUV 2.56 sec
0.05 min End Block
0.05 min Block BufferValve_A1_Inlet

The second logbook line is the ***BatchID*** that is automatically generated.

Autoscroll

The ***Logbook*** pane can autoscroll to display the latest entries. Right-click in the pane, and select ***Autoscroll***. You can also select the ***Autoscroll*** option in the ***Properties*** dialog box (***View: Properties*** and select the ***Logbook*** tab).

How to filter the logbook contents

You can choose to display only selected items in the logbook. The table below describes how to activate the filter.

Step	Action
1	• Right-click in the ***Logbook*** pane and choose ***Properties***. *Result*: The ***Properties*** dialog box opens.
2	• Choose the ***Logbook*** tab. • Select the items you want to display in the logbook (all items are selected by default). • Click the ***OK*** button. *Result*: Only the selected items will be displayed in the logbook. The ***Logbook*** title in the upper right corner will show the text ***(Filter on)*** to indicate that not all items are visible. All items will still be logged in the result file.

How to find logbook text entries

The logbook can be searched for specific text entries. The table below describes the function:

Step	Action
1	Right-click in the ***Logbook*** pane and choose ***Find***. *Result*: The ***Find*** dialog box opens.
2	• Type the text you want to locate. • Select search criteria if necessary. • Click ***OK***. *Result*: The located logbook entry is highlighted.

a

9.3 Manual system control

Introduction

This section describes how to control the system with manual commands and instructions.

In this section

This section contains these topics:

Section	See page
9.3.1 The toolbar and status bar	252
9.3.2 Manual instructions	256
9.3.3 Alarms and warnings	259

9.3.1 The toolbar and status bar

Toolbar buttons

The toolbar at the top of the ***System Control*** module contains three sets of buttons:

- ***Manual Direct Commands*** buttons for starting and stopping the run
- ***Windows*** buttons to access dialog boxes for pane selection, documentation and layout properties
- ***System Access*** buttons to control the system connection.

Show and hide

The toolbars can be shown and hidden by choosing ***View:Toolbars*** and selecting the relevant boxes.

The figure below shows the toolbar:

Manual Direct Commands

The available ***Manual Direct commands*** buttons in ***System Control*** are dependent on the control status of the connection. The table below shows when each button is available:

Control Status	Available buttons
End	***Run***
Running	***Hold***, ***Pause***, ***End***
Manual	***Run***, ***Pause***, ***End***
Hold	***Pause***, ***Continue***, ***End***
Method pause	***Hold***, ***Continue***, ***End***
Manual pause	***Run***, ***Continue***, ***End***

Direct command button functions

The table below describes the functions of the ***Manual direct command*** buttons.

Button	Function
Run	Opens the ***Run*** dialog box, which shows all available methods, as the first step in a method run. If a method is loaded, ***Run Setup*** opens. The run will start immediately if a start protocol isn't part of the method.
Hold	Suspends execution of a method, but continues • to pump liquid at the current flow rate and eluent concentration settings. All settings remain unchanged. • to increase accumulated time and volume. Method instructions are not executed until the ***Continue*** button is pressed.
Pause	Behavior of the ***Pause*** button is strategy-dependent. The ***Pause*** button suspends execution of a method and stops all pumps so that the system comes to a standstill. For ÄKTAdesign systems, valves remain in the position they were in before the pause. Accumulated time and volume is not increased during a ***Pause***. Method instructions are not executed until ***Continue*** is pressed.
Continue	Resumes execution of a paused or held method.
End	• Terminates method execution • Puts the system into an ***End*** state. **Note:** You can choose to save a partial result or discard it.

Note: The commands can also be found on the ***Manual*** menu.

Windows buttons

The table below describes the functions of the ***Windows*** buttons:

Button	Function
	Opens a dialog box where you can choose which window panes to display. This button is equivalent to the menu command ***View:Panes***.
	Opens the documentation pages. Run notes can be entered on the ***Notes*** tab and settings can be changed. Other tabs are displayed for information only. This button is equivalent to the menu command ***View:Documentation***.
	Opens the properties pages. This button is equivalent to the menu command ***View:Properties***.

System Access buttons

There are two functions of the ***System Access*** buttons:

Disconnect/Connect system

The ***Disconnect*** button is used to disconnect the system and leave it in a locked or unlocked state.

The ***Connect*** button connects the system.

Leave/Take control of the system

The ***Leave control*** button leaves the system in a locked or unlocked state.

The ***Take control*** button takes control of the system.

Status bar, connection status

The status bar displays a message indicating the connection status of the window. The table below describes the different messages:

Message	Connection status
Controlled by: <user>	The indicated user has a control mode connection to the system. Other users can establish a view mode connection.
Locked by:<user>	The indicated user has left the system in a locked state. Users who can supply the required password can unlock the system and establish a connection. The password is case sensitive. It is possible to unlock with the "lock" password or with the UNICORN logon password. Anyone who uses the UNICORN logon password must have ***Unlock systems*** access rights. The "lock" password is the password entered by the user who locked the system.
System is available	Any user can establish a connection.

Status bar, Watch status

The status bar displays a message indicating if a ***Watch*** is active in the method.

- Click the ***Active watch*** status message to open the ***Watch*** dialog box with information about the active ***Watch*** instruction.

9.3.2 Manual instructions

Introduction

The chromatography system can be controlled with manual instructions issued from the ***Manual*** menu in the ***System Control*** module. The available instruction options are dependent on the strategy.

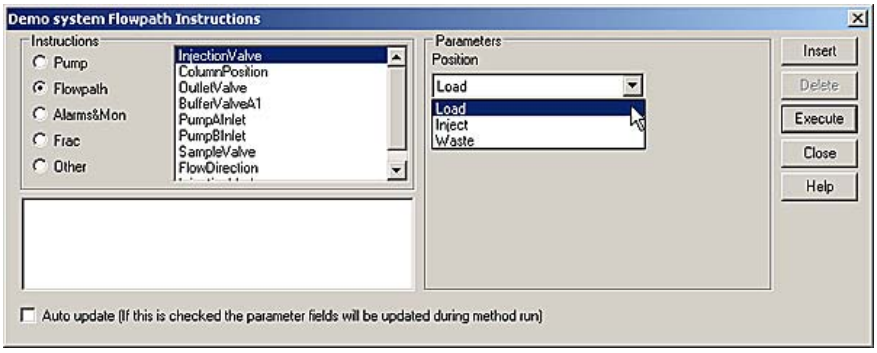
Manual instructions during a method run

Manual instructions can be issued while a method is running. A manual setting applies until the next method instruction of the same type is executed

Example: A manual ***Flow*** instruction will set the flow rate until the next ***Flow*** instruction in the method is executed. Manual instructions that you issue during a method are recorded in the logbook for the method run.

The manual instructions dialog box

The ***Manual*** menu in ***System Control*** opens a dialog box similar to the ***Instruction box*** in the ***Method Editor***. The name of the connected system is displayed on the title bar of the dialog box. See an example in the illustration below:



Note: The parameter values will be updated continually during the run if the ***Auto update*** checkbox is selected.

Column protection

Your user attributes may include a requirement to always set pressure alarms.

Step	Action
1	When you try to execute a pump instruction the ***Column protect mode*** dialog box opens.
2	• Click the ***Yes*** button in the dialog box to select a column and retrieve the correct maximum pressure value. • Click ***OK*** to close the column list. • Click the ***Insert*** button to add the ***Alarm_Pressure*** instruction.
3	• If necessary, repeat step 2 to add an ***Alarm_SamplePressure*** instruction.

How to use manual instructions

Manual instructions are entered in the same way as method instructions from the dialog box in the ***Method Editor***. The table below describes how to add a manual instruction:

Step	Action
1	Select an instruction group and a component in the ***Instructions*** field.
2	Select instruction parameters in the ***Parameters*** field.
3	Click the ***Insert*** or ***Execute*** buttons as needed. (See the descriptions of the different functions below)

The buttons of the manual instructions dialog box

The table below describes the functions of the manual instructions buttons:

Button	Function
Insert	This button places the current instruction in the list at the bottom left of the dialog box.
Delete	This button deletes the selected instruction from the current list only. One instruction can be deleted at a time.

Button	Function
Execute	This button • executes all instructions in the list at the same time or • executes the currently marked instruction if the list is empty. **Note:** Although all instructions are executed simultaneously, some (for example gradient and fraction instructions) may take some time to complete in the liquid handling module.
Close	If you click the ***Close*** button without first clicking the ***Execute*** button, commands in the list • will not be executed • will be deleted from the command list.

How to save manual results

When you choose to run the system manually - as opposed to a ***Method run*** - the results are automatically stored in a folder called ***Manual Runs***. The ***Manual Runs*** folder stores the ten most recent results from your manual runs. To save a result file from the ***Manual Runs*** folder more permanently, you need to move or copy it to another location.

An alternative way to save the results from a manual run is to record the results manually in a result file. The table below shows how to do this:

Step	Action
1	• Choose ***Manual:Other***. • Select the instruction ***Record On*** at the beginning of the run.
2	• Click the ***Execute*** button. *Result*: UNICORN will prompt for a result file name.

9.3.3 Alarms and warnings

Introduction

Alarms and warnings are displayed regardless of the activity currently in progress in UNICORN. You will be notified of an exceeded limit in a running system even if you are developing a method, evaluating data or monitoring a method run on a different system. Warnings and alarms are also recorded in the logbook for the run.

Limits for monitor signals

The system settings determine the acceptable limits of monitor signals during a run. The limits can also be set for the current run by an instruction in the method. Limits set with a method instruction override the limits set in system settings. If these limits are exceeded in a run, a warning or alarm dialog box is displayed on the screen.

Effects of alarms and warnings

Alarms and warnings have different effects on the system:

- *Warning*: The run continues.
- *Alarm*: The system is paused.

In a network system

In a network installation, alarms and warnings are displayed on the controlling station and all stations viewing the system. An alarm can be acknowledged only from the computer connected in control mode. Alarms are displayed but cannot be acknowledged on computers connected in view mode.

9.4 How to perform a scouting run

More information on scouting runs

See *Section 7.1 How to set up a Scouting Scheme, on page 214* for information on how to set up scouting runs.

Instruction

The table below describes how to perform a scouting run:

Step	Action
1	Start the method (see *Section 9.1 How to start a method run, on page 230*). *Result:* The ***Start Protocol*** will display the scouting scheme as defined in the method (assuming that the ***Scouting*** box is selected on the ***Start Protocol*** tab of the ***Run Setup***).
2	Check through the settings for the scouting scheme in the ***Scouting*** tab, and if required, do the following: • Change the scouting variable values. • Right-click the top of the ***Run*** column to toggle the run status between ***Run*** and ***Excluded***.
3	Work through the rest of the ***Start Protocol***. Click the ***Start*** button.

Results of a scouting run

The results of a scouting run are saved in a special scouting folder as defined in the ***Results*** tab of the ***Start Protocol***. Within the folder, each run is saved in a separate result file named according to the usual naming rules (see *Section 6.5.12 The Result Name tab, on page 180*).

If the ***Start Protocol*** is displayed for each run in a scouting scheme, you are able to change the result file name during scheme execution.

How to change scouting variables during a run

- At any time during a run, you can click the ***View Documentation*** icon in ***System Control*** and change the scouting variables on the ***Scouting*** tab for runs which have not yet been started.

- Settings for the run that is currently in progress cannot be changed.
- You can add more scouting runs to the scheme as long as the last run has not been started.
- You can use this feature to adjust variables for scouting even if the start protocol is not displayed at the beginning of each run.

9.5 How to perform a MethodQueue run

Instruction

The table below describes how to run a ***MethodQueue***:

Step	Action
1	• Make sure that all systems used in the ***MethodQueue*** are connected with control mode connections.
2	Select a ***MethodQueue*** in the ***Methods*** pane in the ***UNICORN Manager*** and • choose ***File:Run*** *or* • right-click the ***MethodQueue*** icon in the ***Methods*** pane and select ***Run*** from the shortcut menu. *or* • double-click the ***MethodQueue*** icon in the ***Methods*** pane and click the ***Run*** button in the ***MethodQueue Editor*** dialog box. *Result:* The ***MethodQueue*** will start in accordance with the conditions defined in the ***MethodQueue*** setup.

See *Section 8.1 How to create a new MethodQueue, on page 222* for information about how to create a ***MethodQueue***.

Unattended MethodQueue operation

The ***Start Protocol*** for the first and each subsequent method step in the ***MethodQueue*** is displayed when the corresponding method is run. If you require unattended ***MethodQueue*** operation after the start of the first method step, make sure that subsequent method steps do not include a ***Start Protocol***.

Note: If the ***Start Protocol*** for a method in the queue is cancelled, the ***MethodQueue*** is paused. Select ***MethodQueue:Display Running*** in the ***UNICORN Manager*** and ***Restart*** or ***End*** the run in the displayed dialog box.

MethodQueues when the system is busy

You can choose to place a method in a ***MethodQueue*** if the system is already busy with another method run (See *Section 8.1 How to create a new MethodQueue, on page 222*). In a similar manner you can also start a new ***MethodQueue*** while another ***MethodQueue*** is in progress. It will be placed in queue and executed when the first queue is completed.

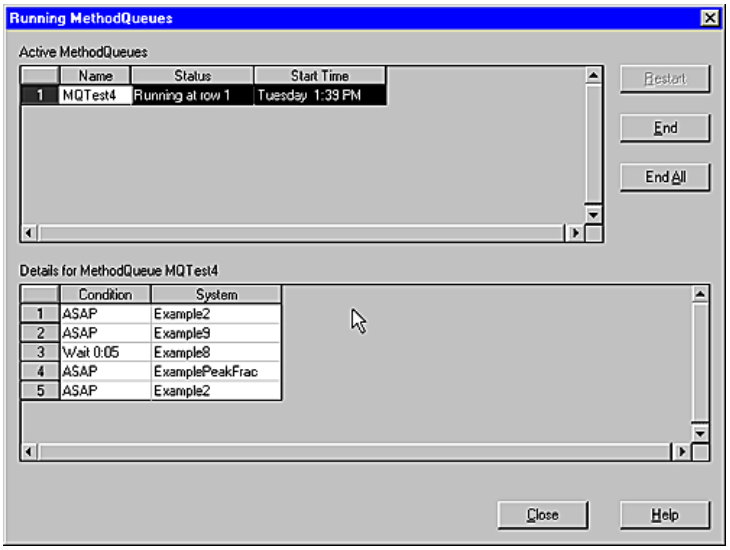
How to display and edit pending and running MethodQueues

Definition: A pending ***MethodQueue*** is one for which ***Run*** has been requested but which has not yet started, either because the system is not available or because the setup time has not been reached.

The table describes how to display running and pending ***MethodQueues***.

Step	Action
1	Click the ***Running MethodQueue*** icon.

Result: The ***Running MethodQueue*** dialog box is displayed.



Step	Action
2	Select a ***MethodQueue*** in the ***Active MethodQueues*** list box. *Result:* Information on the selected ***MethodQueue*** is displayed in the ***Details for...*** field of the dialog box. **Choose from the following:** • The ***Restart*** button restarts the currently running ***MethodQueue*** if a ***Start Protocol*** has been terminated by ***Cancel***. • The ***End*** button terminates a running ***MethodQueue*** after the current step. Any methods currently in operation will continue to run and must be terminated with the ***End*** button in the ***System Control*** window if they are not to run to completion. If you click the ***End*** button for a pending ***MethodQueue***, it is deleted from the pending list. • The ***End All*** button terminates the running ***MethodQueue*** and deletes all ***MethodQueues*** from the pending list. • The ***Close*** button closes the dialog box.

9.6 If the network connection fails

Results will be saved in the Failed folder

If the results of a method run are stored on a server or other location, and there is a network communication failure during a method run that has been started from a remote station, the method run will continue and the results will be saved in the ***Failed*** folder on the local station. A control mode connection can be established on the local station to control the running system. See the Administration and Technical Manual for more details.

10 How to view results

Introduction

A result file is automatically generated at the end of a method run and contains a complete record of the method run, including method, system settings, curve data and method run log. The ***Evaluation*** module offers facilities for presentation and evaluation of curve data.

This chapter describes how to present the chromatograms and curves of your result file and how to create and print reports.

In this chapter

This chapter contains these sections:

Section	See page
10.1 How to open a result file	267
10.2 How to use the File Navigator	269
10.3 Basic presentation of chromatograms	275
10.4 How to optimize the presentation of a chromatogram	285
10.5 How to print active chromatograms	300
10.6 How to create and print reports	302
10.7 Run documentation	327

10.1 How to open a result file

Introduction

All contents of the result files are opened in the ***Evaluation*** module. By default, the chromatograms in a run are shown as opened windows. The chromatogram window on top is the active window.

There is also a minimized ***Temporary*** chromatogram window.

See *Section 10.3 Basic presentation of chromatograms, on page 275* for further information about chromatograms.

Note: It is not possible to open the same result file from two different locations simultaneously.

How to open a result from the UNICORN Manager

To open a result file from the ***UNICORN Manager***, do one of the following:

- Double-click a result file in the ***Results*** window of the ***UNICORN Manager***,

  or

- Select a result file icon in the ***Results*** window of the ***UNICORN Manager*** and select ***File:Open***,

  or

- Click the ***Evaluation*** icon in the ***UNICORN Manager***, open the ***Evaluation*** module and select a result file from the ***Open Result*** dialog box.

How to open a result in the Evaluation module

To open a result file in the ***Evaluation*** module:

- Do the following:
  - Select ***File:Open***
  - Select a result file from the ***Open Result*** dialog box.

or

- Do the following:
  - Select ***View:File Navigator***
  - Locate and select a result file from the ***File Navigator***.

Note: See *Section 10.2 How to use the File Navigator, on page 269* for detailed instructions on how to locate files and set up File Navigator preferences.

10.2 How to use the File Navigator

Introduction

The ***File Navigator*** can be used to locate and open result files in the ***Evaluation*** module. Recent runs are also listed based on the user preferences.

How to open the File Navigator

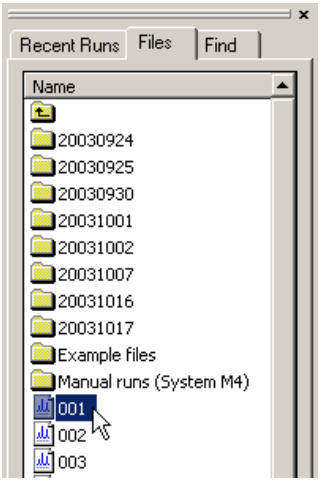
To open the ***File Navigator***:

- Click the ***Evaluation*** module icon in the Windows task bar.
- Select ***View:File Navigator***

Result: The ***File Navigator*** opens in the ***Evaluation*** module. The ***File Navigator*** can be resized and dragged to other positions in the module.

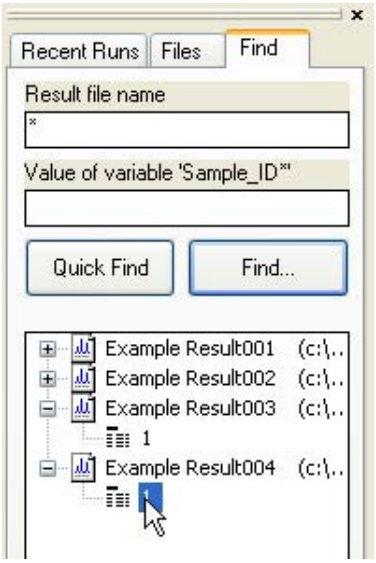
How to open files from the Files list

The table below describes how to use the ***Files*** list to locate and open a result file.

Step	Action
1	• Click the ***Files*** tab *Result*: The ***Files*** list opens in the ***File Navigator***. The list is identical to the ***Results*** window in the ***UNICORN Manager*** and shows all user available folders and files. 
2	• Navigate to the desired folder • Double-click the desired result file *Result*: The result file opens in the ***Evaluation*** module.

How to use Find to search for files

The ***Find*** function in the File Navigator is used to locate result files in the available folders. The table below describes how to use the ***Find*** function to locate and open a result file.

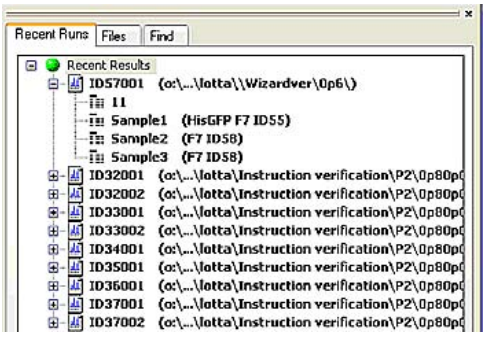
Step	Action
1	• Click the ***Find*** tab *Result*: The ***Find*** list opens in the ***File Navigator***. 
2	• Type a file name or part of a file name in the ***Result file name*** text box. Standard wildcard characters can be used. *or* • Type a Sample ID value in the ***Value of variable Sample_ID*** text box. **Note:** The defined variable name must begin with ***Sample_ ID***.
3	• Click the ***Quick Find*** button *Result*: The located result files are listed in the ***File Navigator***.
4	• Double-click the desired result file or chromatogram *Result*: The file or chromatogram opens in the ***Evaluation*** module.

Note: Click the ***Find*** button to open the ***Find Files*** dialog box where more search functions are available. See *Section 4.3 How to arrange and locate your files, on page 88* for more information.

How to open a Recent Run

The ***Recent Runs*** list shows all the available recorded recent runs based on the selected user preferences. The table below describes how to use the ***Recent Runs*** list to locate and open a result file.

Step	Action
1	• Click the ***Recent Runs*** tab *Result*: The ***Recent Runs*** list opens in the ***File Navigator***.



Note: Until the files and chromatograms in the list have been opened and saved they are noted in bold text. When they are opened and saved the text is changed to plain text.

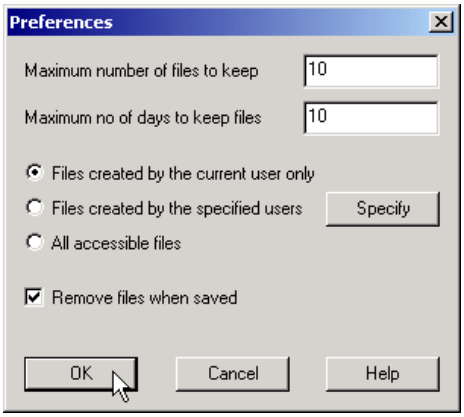
2	• If needed, click the ***Refresh*** button in the bottom of the ***File Navigator*** *Result*: The ***Recent Runs*** list is updated with all runs that were performed since the ***File Navigator*** was opened the last time.
3	• Locate the desired run • Double-click the file *Result*: The result file opens in the ***Evaluation*** module.

Note: Click the **+** signs to view or select individual chromatograms from the result files. Individual result files can be selected and removed from the list by clicking the ***Remove*** button. The ***Remove all*** button clears the whole list.

Note: ***Remove*** only clears the list, the files are not deleted.

How to set preferences for Recent Runs

The ***File Navigator*** will display ***Recent Runs*** based on the individual user preference settings. The table below describes how to adjust the preference settings:

Step	Action
1	• Click the ***Preferences*** button *Result*: The ***Preferences*** dialog box opens. 
2	• Type the maximum number of files to keep on the list • Type the maximum number of days to keep the files on the list
3	Select which files to display on the list: • Only files created by the current user • All files created by specified users **Note:** Click the ***Specify*** button to open a dialog box and select from a list with all accessible users. • All accessible files regardless of the creator
4	• Choose ***Remove files when saved*** if the files are to be removed from the list when they have been saved. • Click the ***OK*** button. *Result*: All new results will be displayed on the ***Recent Runs*** list based on the changed preferences.

How to close the File Navigator

To close the ***File Navigator***:

- Click the small cross in the top right-hand corner of the ***File Navigator***.

Result: The ***File Navigator*** closes.

10.3 Basic presentation of chromatograms

Introduction

This section describes how to access result files and optimize the presentation of a chromatogram and its curves via the ***Chromatogram Layout*** dialog box.

In this section

This section contains these topics:

Section	See page
10.3.1 Introduction and temporary chromatograms	276
10.3.2 The chromatogram window	278

10.3.1 Introduction and temporary chromatograms

Contents of a chromatogram

Chromatograms can be viewed in the ***Evaluation*** module.

A chromatogram includes a number of curves that have been created during a method run, such as UV, conductivity, pH, fraction marks, etc. A chromatogram also contains the curves created and saved during an evaluation session. The original raw data curves cannot be deleted or modified, but they can be used as the basis for evaluation procedures and subsequent creation of new curves.

Temporary chromatograms

A ***Temporary*** chromatogram is essentially an empty chromatogram that is specific to the ***Evaluation*** module. It is also user-specific, so that all users have their own.

Information contained within a ***Temporary*** chromatogram is automatically saved from one evaluation session to the next, but is not saved within the result files.

How to copy curves into Temporary

Curves can be copied into ***Temporary*** and comparisons or evaluations can be performed. This is particularly useful if you do not want to clutter up your original chromatograms with a large number of curves. It can also be used to keep blank run curves or curves to compare when you open different result files.

The table below describes how to copy curves into ***Temporary***:

Step	Action
1	Open a result file.
2	Select ***Edit:Copy:Curves.*** *Result:* The ***Copy Curve*** dialog box is displayed.
3	Select a source chromatogram and a curve to be copied in the ***Source Chromatogram*** fields.
4	Select ***Temporary*** as the target chromatogram and a position for the new curve in the ***Target Chromatogram*** fields.

Step	Action
5	Click the ***Copy*** button. *Result:* The curve is copied into the ***Temporary*** chromatogram. Click the ***Close*** button.

How to clear a temporary chromatogram

The table below describes how to clear the contents of a temporary chromatogram:

Step	Action
1	Open the relevant result file.
2	• Select ***Edit:Clear Temporary Chromatogram***. • Click the ***Yes*** button to confirm.

10.3.2 The chromatogram window

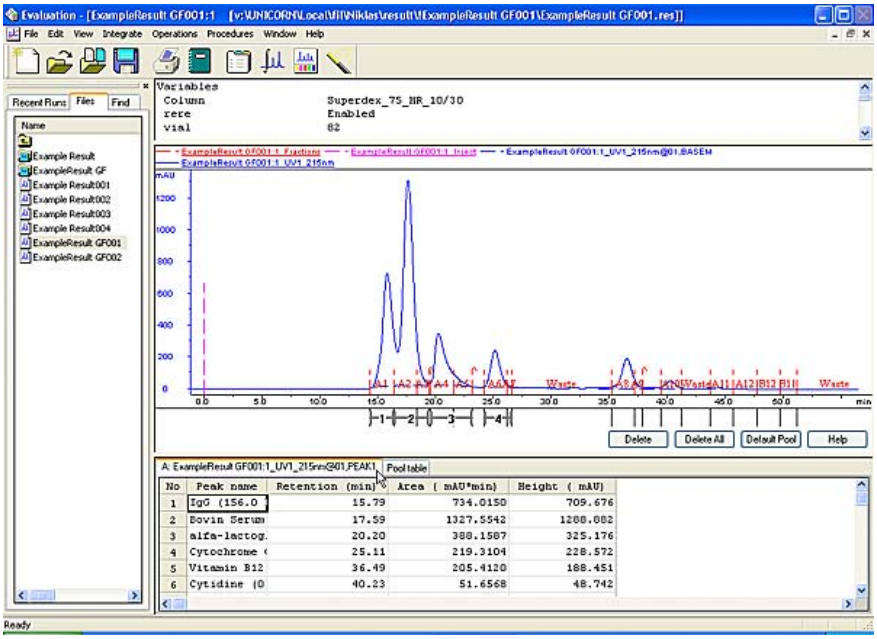
Main views

The chromatogram window is divided into four main views:

- File Navigator
- header information
- curves
- peak and pool tables

The displayed areas for the views can be adjusted by dragging the borders with the mouse cursor between the views.

The picture below shows an example of the window with all views present:



How to view header information

You can display header information at the top of a chromatogram, with details on variables, scouting variables, questions and/or notes. Header information cannot be displayed for imported chromatograms.

The table below describes how to display header information:

Step	Action
1	Open a result file.
2	In the ***Evaluation*** module, select ***Edit:Chromatogram Layout...*** *Result:* The ***Chromatogram Layout*** dialog box is displayed.
3	• Click the ***Header*** tab. • Select the options you want in the header. • Click ***OK***.
4	• In the chromatogram window, place the cursor at the top of the curve window (just below the toolbar) until the window sizing tool appears. • Drag the cursor down to display the header window.

How to view peak table information

The table below describes how to display peak table information if the result has been integrated:

Step	Action
1	Open a result file.
2	• Choose ***Edit: Chromatogram Layout***. *Result:* The ***Chromatogram Layout*** dialog box opens.
3	• Click the ***Peak Table*** tab. • Select a peak table in the ***Select peak table to display*** list. • Select what peak table columns to display. • Check if global peak table data should be displayed or not. • Click ***OK***.

How to view the Pool table

If fractions are pooled, the ***Pool Table*** is displayed in the same pane as the ***Peak Table***.

- Click the ***Pool Table*** tab to display the ***Pool Table*** information.

See *Section 11.5 How to pool fractions, on page 340* for more information on how to create the ***Pool Table***.

Run curves, default appearance and information

The first time a result file is opened and viewed, a default layout is applied to display all the original curves. The default layout can be changed by the user (see *Section 10.4.5 How to save and apply a layout, on page 294*).

Information for each curve

Each curve is automatically assigned a default color and style, with default information about each curve displayed in the key above the curves. This information includes

- result file name
- chromatogram name
- curve name.

Choose the Y-axis scale

Each curve has a correspondingly colored Y-axis. To choose the appropriate Y-axis scale

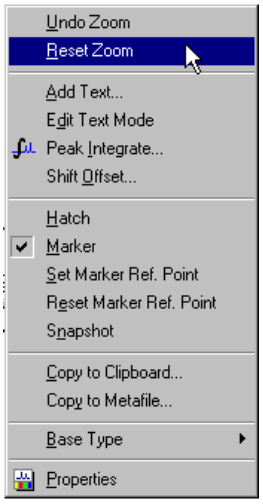
- click on the Y-axis until the desired scale is displayed

or

- click on the name of the curve.

Run curves, shortcut menu

When viewing curves in the ***Evaluation*** module, you can access a menu that provides a quick alternative to menu commands. Right-click the run curves view to display the menu shown in the picture below:



Optimizing the workspace

The chromatogram window can be minimized and maximized using ordinary Windows commands. The table below describes extra features to optimize the workspace:

Use the command	if you want...
Window:Arrange icons	to arrange icons of minimized windows.
Window:Tile	to view several chromatogram windows side by side.
Window:Cascade	to stack the open windows like a deck of cards.

How to display a vertical marker line

The table below describes how to display a vertical marker line:

Step	Action
1	Right-click the ***Curves*** pane and select ***Marker***.
2	Drag the marker line with the mouse. *Result:* Where the line bisects the curve, the X-axis and Y-axis values are displayed at the top right corner of the pane.

Note: Right-click and select ***Snapshot*** to record the marker position values. See *Section 2.2.7 Snapshots, on page 50* for more information about the ***Snapshot*** function.

How to set a reference point

The table describes how to set a reference point:

Step	Action
1	• Display a ***Marker*** in the ***Curves*** pane. • Right-click and select ***Set Marker Ref. Point*** to define a reference point for the marker position.
2	When the marker is moved from the reference point, the X-axis and Y-axis values for the new position are displayed together with: • the new position in relation to the reference point, • the minimum, maximum and average values for the curve interval between the reference point and the new position.

How to display the logbook overlay

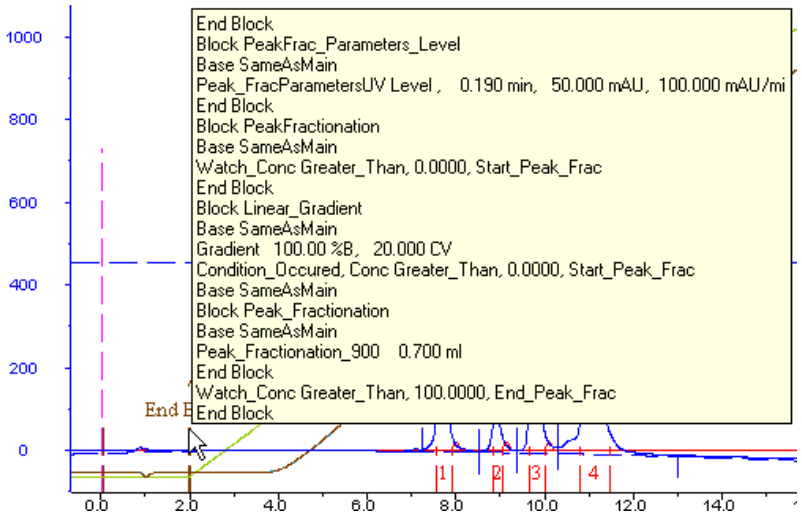
The table below describes how to display the logbook entries as an overlay in the chromatogram.

Step	Action
1	• Right-click in the chromatogram window and choose ***Properties*** on the shortcut menu. *Result*: The ***Chromatogram Layout*** dialog box opens.
2	• Choose the ***Curve*** tab. • Select the ***Logbook*** curve.
3	• Choose the ***Curve Style and Color*** tab. • Click the ***Filter*** button in the ***Logbook text alignment*** field. *Result*: The ***Filter Logbook*** dialog box opens.
4	• Select all the logbook items you want to display and click ***OK***. • Click ***OK*** in the ***Chromatogram Layout*** dialog box. *Result*: The selected logbook items are displayed in the chromatogram window.

How to view the complete logbook information

At some breakpoints there can be more logbook information than what is possible to conveniently display in the chromatogram window. The additional information that is not displayed is indicated by an arrow point symbol by the break point.

- Hold the mouse cursor over the break point to display the complete information in a flyover text box, as shown in the illustration below:


End Block
Block PeakFrac_Parameters_Level
Base SameAsMain
Peak_FracParametersUV Level , 0.190 min, 50.000 mAU, 100.000 mAU/mi
End Block
Block PeakFractionation
Base SameAsMain
Watch_Conc Greater_Than, 0.0000, Start_Peak_Frac
End Block
Block Linear_Gradient
Base SameAsMain
Gradient 100.00 %B, 20.000 CV
Condition_Occured, Conc Greater_Than, 0.0000, Start_Peak_Frac
Base SameAsMain
Block Peak_Fractionation
Base SameAsMain
Peak_Fractionation_900 0.700 ml
End Block
Watch_Conc Greater_Than, 100.0000, End_Peak_Frac
End Block
1000
800
600
400
200
0
0.0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
1
2
3
4

10.4 How to optimize the presentation of a chromatogram

Introduction

This section describes some of the ways you can optimize the presentation of a chromatogram.

In this section

This section contains these sub-sections:

Section	See page
10.4.1 How to make changes in the Chromatogram Layout dialog box	286
10.4.2 The Curve tab and Curve Names tab	287
10.4.3 The Curve Style and Color tab	289
10.4.4 How to change and fix the axes	292
10.4.5 How to save and apply a layout	294
10.4.6 How to show part of a curve	296
10.4.7 How to change the size of Fraction, Injection and Logbook marks	299

10.4.1 How to make changes in the Chromatogram Layout dialog box

Instruction

The ***Chromatogram Layout*** dialog box is used to make changes regarding chromatogram presentation. The main features of the ***Chromatogram Layout*** dialog box regarding chromatograms are described in the subsequent sections in this chapter.

Features regarding peak tables are described in *Section 12.1.2 How to perform a peak integration, on page 403*.

The table below describes how to make changes in the ***Chromatogram Layout*** dialog box:

Step	Action
1	Open a result file.
2	• Right-click the chromatogram window and select ***Properties*** *or* • Choose ***Edit:Chromatogram Layout***. *Result:* The ***Chromatogram Layout*** dialog box is displayed. The view from which you activate the ***Properties*** command determines the tab that is displayed in the ***Chromatogram Layout*** dialog box.
3	Carry out the changes on the different tabs to get the desired layout for header, curves and peak table. Select ***Apply to all chromatograms*** if you want to apply changes made in the ***Chromatogram Layout*** dialog box to all open chromatograms. Click ***OK***.

10.4.2 The Curve tab and Curve Names tab

The Curve tab

The ***Curve*** tab of the ***Chromatogram Layout*** dialog box contains a list of all the curves included in the chromatogram. Select the curves you want to display in the chromatogram, and click ***OK***.

Curve name appearance

You select options for the curve name appearance on the ***Curve Names*** tab. This is an example of a default curve name:

Result:11_UV1_280

The table below describes the three components that make up the default curve name:

Component	Description	Example
Result name	Name of the result.	Result
Chromatogram name	Number given automatically during a run or a name defined by the ***New_Chromatogram*** instruction.	11
Curve name	Curve type, for example detection of an eluted component. In this example, the system uses a variable wavelength detector, so the wavelength (280) for the UV curve is also given.	UV1_280

How to choose curve name appearance

You can choose to view only part of the curve name. The table below describes how to do this:

Step	Action
1	Open a result file.
2	Choose ***Edit:Chromatogram Layout***. *Result:* The ***Chromatogram Layout*** dialog box is displayed.

Step	Action
3	Click the ***Curve Names*** tab.
4	• Select the appropriate boxes for ***Curve name appearance***. • Select the appropriate ***Curve legend position***. • Click ***OK***.

Note: It is usually sufficient to select the ***Curve Name*** option if only one chromatogram is being evaluated. However, confusion can arise when more than one chromatogram is shown, so more complete names might be necessary.

10.4.3 The Curve Style and Color tab

Introduction

All curves within a chromatogram are represented by a default color and line style. Curves imported into the chromatogram or newly created curves are automatically assigned a color and line style.

Peak label settings

Peaks can be labeled on the ***Curve Style and Color*** tab of the ***Chromatogram Layout*** dialog box. Use a combination of the following labels:

- ***Retention*** (the default label)
- sequential ***Number***
- user-defined ***Peak name***.

Fraction text and Logbook text alignment settings

Both ***Fraction text*** and ***Logbook text*** can be set to the following alignment options:

- ***Vertical***
- ***Horizontal***
- ***Fly Over***, which sets text labels as hidden text that appears only when the cursor is carefully positioned over a fraction mark.

How to change the color and style of a curve

The table below describes how to change the color and style of a curve:

Step	Action
1	Open a result file.
2	Choose ***Edit:Chromatogram Layout***. *Result:* The ***Chromatogram Layout*** dialog box is displayed.
3	Click the ***Curve Style and Color*** tab.

Step	Action
4	• Select the curve you want to change from the list. • Select the desired color and style. • Click ***OK***.

How to display and filter logbook information

The table below describes how to display and filter logbook curve information:

Step	Action
1	Open a result file.
2	• Choose ***Edit:Chromatogram Layout***. *Result:* The ***Chromatogram Layout*** dialog box is displayed.
3	• Click the ***Curve*** tab. • Select the logbook curve.
4	• Click the ***Curve Style and Color*** tab. • Click the ***Filter...*** button in the ***Logbook text alignment*** field. *Result:* The ***Filter Logbook*** dialog box is displayed.
5	• Select the type of logbook information you want to show. • Set the maximum block depth to show. • Click ***OK***.

How to display a hatched background

The table below describes how to display a hatched background in the chromatogram window:

Step	Action
1	Open a result file.
2	• Choose ***Edit:Chromatogram Layout***. *Result:* The ***Chromatogram Layout*** dialog box is displayed.
3	• Click the ***Curve Style and Color*** tab. • Select the ***Hatch*** box. • If desired, select the ***Apply to all chromatograms*** box and click ***OK***. *Result:* Hatch marks are displayed as a background.

Note: You can also right-click in the ***Chromatogram*** window and select ***Hatch***.

10.4.4 How to change and fix the axes

How to change and fix the Y-axis

The table below describes how to change and fix the Y-axis:

Step	Action
1	Open a result file.
2	Choose ***Edit:Chromatogram Layout***. *Result:* The ***Chromatogram Layout*** dialog box is displayed.
3	Click the ***Y-Axis*** tab.
4	• Select the appropriate curve from the list. • Click the ***Fixed*** option.
5	• Type the desired minimum and maximum values. • Click the ***All with this unit*** button if you want other curves with the same Y-axis units as the current scaled curve to be similarly scaled. **Note:** The values will only be applied to existing curves. They will not be applied to new curves created after this function was last used. • Click the appropriate ***Pressure unit*** (***MPa***, ***psi***, ***bar***) option to change Y-axis units for pressure curves. **Note:** Default ***Pressure unit*** is ***From strategy***, which is the unit defined in the original run strategy. • Click ***OK***.

How to add a second Y-axis

The table below describes how to add a second Y-axis to the chromatogram.

Step	Action
1	Choose ***Edit:Chromatogram Layout***. *Result:* The ***Chromatogram Layout*** dialog box is displayed.
2	Click the ***Y-Axis*** tab.

Step	Action
3	• Select the appropriate curve from the ***Right Axis*** droplist. • Click the ***OK*** button.

How to change and fix the X-axis

The table below describes how to change and fix the X-axis:

Step	Action
1	Open a result file.
2	Choose ***Edit:Chromatogram Layout***. *Result:* The ***Chromatogram Layout*** dialog box is displayed.
3	Click the ***X-Axis*** tab.
4	Select the appropriate option in the ***Base*** field: • ***Time*** of retention • ***Volume*** • ***Column Volume*** **Note:** Some calculated curves, for example baselines, exist in only one base and might seem to disappear when the base is changed. Curves are collected in time and recalculated for display in volume. Thus, switching the base between ***Time*** and ***Volume*** can slightly alter the resolution.
5	• Click the ***Fixed*** option in the ***Axis scale*** field to set the axis limits manually. • Type the desired minimum and maximum values. • If desired, de-select the ***Adjust retention zero to injection number*** checkbox. This checkbox is selected by default. The function sets the time/volume to zero at the injection mark, that is when the sample was injected. The time and volume before injection will become negative values. • Click ***OK***.

10.4.5 How to save and apply a layout

Introduction

All configurations that you make in the ***Chromatogram Layout*** dialog box can be saved as a layout. It is possible to apply saved layouts to other chromatograms. All saved layouts are user-specific.

How to save a layout

The table below describes how to save a layout:

Step	Action
1	Open a result file.
2	Choose ***Edit:Chromatogram Layout***. *Result*: The ***Chromatogram Layout*** dialog box is displayed.
3	Make the appropriate layout configuration within the various tabs. **View your changes** Click ***OK*** if you want to return to the chromatogram window to see the applied affects of a given configuration. Return to the ***Chromatogram Layout*** dialog box to perform further changes.
4	• Select the ***Layout Library*** tab. • Click the ***Save current layout as*** button. *Result:* The ***Save Layout*** dialog box is displayed.
5	• Type a name for the layout. • If you want the current layout to be the new default layout, select the ***Save as default*** option. • Click ***OK***. *Result:* The new name is added to the ***Saved layouts*** list.
6	Click ***OK***.

How to apply a layout

The table below describes how to apply a layout:

Step	Action
1	Select the ***Layout Library*** tab on the ***Chromatogram Layout*** dialog box.
2	• Select a layout from the ***Saved layouts*** list. • Click the ***Apply selected layout*** button. *Result:* The layout is automatically applied to the active chromatogram window.
3	If the same layout is to be applied to all chromatograms on the ***Evaluation*** workspace, select the ***Apply to all chromatograms*** checkbox.
4	Click ***OK***.

10.4.6 How to show part of a curve

Introduction

You can select a part of a curve in order to examine details more closely.

You can

- use the zoom to magnify

  or

- cut the axes.

It is also possible to fix the axes, see *Section 10.4.4 How to change and fix the axes, on page 292*.

How to use the zoom function

In the active chromatogram window, you can zoom in on a designated area of the chromatogram. This is the easiest and quickest way to enlarge different parts of a curve. The table below describes how to do this:

Step	Action
1	Open a result file.
2	• Place the mouse pointer in any corner of the area you want to magnify. • Press and hold the left mouse button. A magnifying glass icon will be added to the mouse pointer arrow on the screen. • Drag a box to cover the area to be magnified, and release the mouse button. *Result:* The selected region is now displayed in the entire chromatogram window, together with appropriate scales for the Y and X axes.
3	Use the arrow keys on the keyboard to move around in the chromatogram at the current zoom scale.
4	**Undo zoom** Right-click in the window and select ***Undo zoom*** to undo the last zoom step. **Reset zoom** Right-click in the window and select ***Reset zoom*** to reset all zoom steps at once.

How to cut a curve and store as a new curve

The table below describes how to cut the curve between two values on the X-axis and store this part of the curve as a new curve:

Step	Action
1	Open a result file.
2	Choose ***Operations:Cut curve***. *Result*: The ***Select Curve(s) to Operate On*** dialog box opens.
3	• Select the curves to be operated on. • Click ***OK***. *Result:* The selected curves are shown in the ***Cut*** dialog box which contains two vertical cursor lines.
4	To select the region to be cut, either • drag the two cursor lines to define the left and right limits of the cut area *or* • type the desired left and right limit values in the ***Left limit*** and ***Right limit*** boxes. **Note:** The areas outside of the ***Left limit*** and ***Right limit*** will not be saved in the newly created cut curve. Thus, the X-axis of the new curve will not begin at zero unless this is designated as one of the limits. The original curve is not changed.
5	Click ***OK***. *Result:* The ***Save Cut Curves*** dialog box opens.
6	• Select whether to save the new cut curve in - the ***Source chromatogram***, that is the current active chromatogram, *or* - a ***New chromatogram*** (if you select this option, you can change the name of the chromatogram. Note that it is a recommendation not to use only numbers as names for chromatograms.).

Step	Action
7	Click ***OK***. *Result:* • If the destination of the cut curve was the source chromatogram, the cut curve is automatically displayed in the source chromatogram. • If the destination of the cut curve was a new chromatogram, this will be represented as a new, open chromatogram window.

10.4.7 How to change the size of Fraction, Injection and Logbook marks

Introduction

The sizes of ***Fraction***, ***Injection*** and ***Logbook*** marks are all determined by your user settings. The settings are applied for all your chromatograms.

Instruction

The table below describes how to change the size of the ***Fraction***, ***Injection*** and ***Logbook*** marks:

Step	Action
1	• Choose ***Administration:Change User Attributes*** in the ***UNICORN Manager*** module. *Result*: The ***Change user attributes*** dialog box opens.
2	Select the unit for the ***Fraction mark height***: • ***Percent of window height*** • ***Character Heights*** • ***Pixels*** Type a new size value in the ***Fraction mark height*** box.
3	• Repeat step 2 for the ***Injection*** and ***Logbook*** marks if necessary. • Click ***OK***.

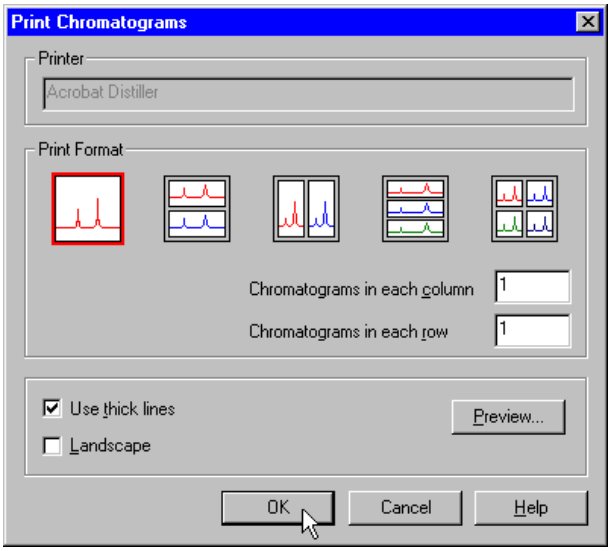
10.5 How to print active chromatograms

Introduction

This section describes how to print the chromatograms that are open in the ***Evaluation*** module.

The Print Chromatograms dialog box

This is an illustration of the ***Print Chromatograms*** dialog box.
Note: The selected print format is outlined in red.



Instruction

The table below describes how to print active chromatograms on the default Windows printer.

Step	Action
1	Open all chromatograms that you want to print in the ***Evaluation*** module.

Step	Action
2	• Select ***File:Print***. *or* • Click the ***Print*** toolbar icon. *Result*: The ***Print Chromatograms*** dialog box opens.
3	Select print format and layout options.
4	• Click ***OK*** to print. *or* • Proceed with step 5 to preview and edit the layout.
5	Click the ***Preview*** button. Result: The ***Customize Report*** window opens.
6	• Click the ***Edit Mode*** button to make changes, e.g. change the order of the chromatograms (see *Section 10.6.1 How to create and print a customized report, on page 303* for more information about how to edit). • Click the ***Preview*** button to return to preview mode.
7	• Select ***File:Print***. *or* • Click the ***Print*** toolbar icon. *Result*: The ***Print*** dialog box opens.
8	• Select the print range and number of copies. • Click ***OK***.

10.6 How to create and print reports

Introduction

The ***Evaluation*** module provides extensive tools to create detailed reports. This section describes how to create and print reports that are based either on a standard or a customized layout.

In this section

This section contains these topics.

Section	See page
10.6.1 How to create and print a customized report	303
10.6.2 How to create and print a standard report	320
10.6.3 How to edit an existing report format	324

10.6.1 How to create and print a customized report

Introduction

You can choose from a variety of objects to include in a report, including chromatograms, methods, documentation, free text and more in the customized report interface. You can also place, align and size the objects as you please. This section describes how to create a customized report format.

Should you need to store store your reports in an electronic format you can save them as PDF files. This section also describes how to do this.

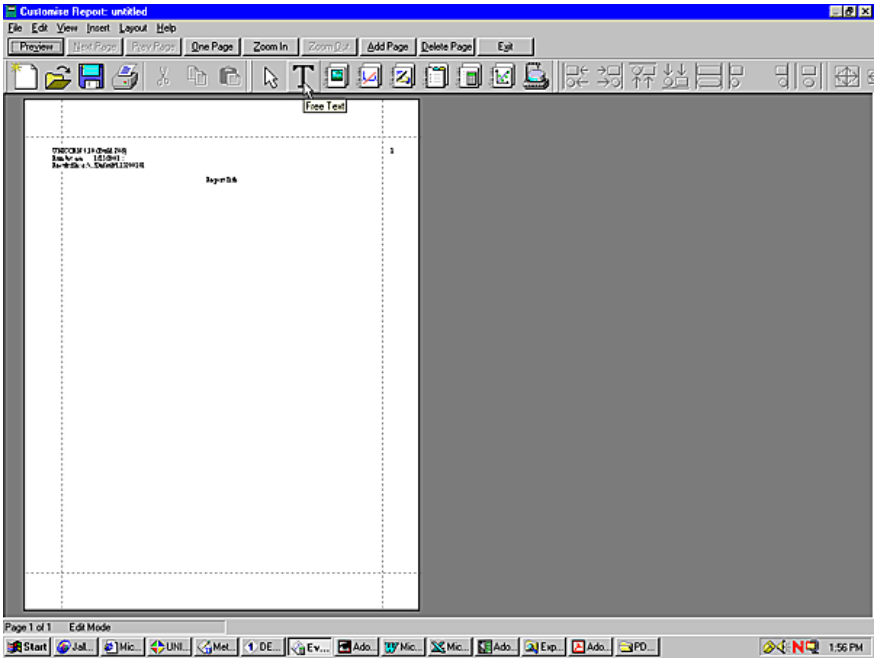
How to open the Report Editor in edit mode

The table below describes how to open the ***Report Editor*** in ***Edit mode*** to create a customized report format.

Step	Action
1	Open a result file in the ***Evaluation*** module.
2	• Select ***File:Report***. *or* • Click the ***Report*** icon. *Result*: The ***Generate Report*** dialog box opens.
3	• Click the ***New*** button. *Result*: The ***Create New Report Format*** dialog box opens.
4	• Select the ***Customized format*** and click ***OK***. *Result*: The ***Report Editor*** opens in ***Edit mode***.

The Edit mode window

The illustration below shows the ***Report Editor*** window in ***Edit mode*** with a blank report open:



Toolbar button functions in the Report Editor

The table below describes the different functions of the Edit mode toolbar buttons in the ***Report Editor***:

Toolbar button	Function
Preview/Edit	This button toggles between a print preview of the report and the ***Edit mode***.
Next Page	This button displays the next page or pair of pages (where there are more than one page).
Prev Page	This button displays the previous page or pair of pages (where there are more than one page).

Toolbar button	Function
One Page/Two Pages	This button toggles between single page view and pairs of pages view, when there is more than one page.
Zoom In	This button increases the magnification of the view.
Zoom Out	This button decreases the magnification of the view.
Add Page	This button adds a blank page to the report.
Delete Page	This button deletes the current page from the report.
Exit	This button closes the ***Customize Report*** window.

How to add and delete report pages

The table below describes how to add or delete report pages in the ***Report Editor***:

If you want...	then...
to add new pages,	• click the ***Add Page*** toolbar button. *Result*: A new page is added after the last page.
to delete a page while in ***One Page*** mode,	• select the page with ***Next Page*** or ***Prev Page***, • click the ***Delete Page*** toolbar button and confirm the deletion.
to delete a page in ***Two Page*** mode,	• select the page with ***Next Page*** or ***Prev Page***, • click an object on the page, • click the ***Delete Page*** toolbar button and confirm the deletion.

How to change the page layout

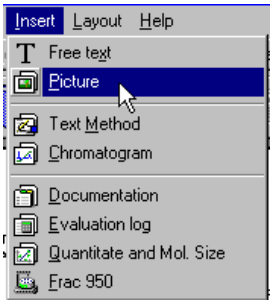
The page layout is changed in the ***Page Setup*** dialog box. The table below describes how to set up the page layout:

Step	Action
1	Double-click anywhere on the report page in the ***Report Editor*** (not on an object). *Result*: The ***Page Setup*** dialog box opens.
2	• Type new values for the ***Margins*** if necessary. • Select the appropriate ***Settings*** and ***Unit***.
3	• Click the ***First Header*** tab. **Note:** An extra ***Header*** tab will appear if you de-select the option to have the same header on all pages. The ***First Header*** tab is used for the first page header only, and the ***Header*** tab is used for all subsequent pages. • Select all the items you want to include in the header from the ***Select Items*** list. • Click the ***Font*** button to change the font for all items if necessary.
4	• Type header text in the ***Free text*** box and click the ***Font*** button to alter the default font if necessary. • Type the report title in the ***Report title*** box and click the ***Font*** button to alter the default font if necessary.
5	• Select the ***Logo*** check box and click the ***Browse*** button if you want to locate and select a logo image file. • Select the ***Alignment*** for the logo, if necessary. **Note:** The logo file must be in bitmap format (***.bmp***) and smaller than 64 kB. Larger logo files or files in other formats must be inserted as ***Picture*** objects.
6	If you want to have a line under or over the header, select the appropriate option in the ***Layout*** field.
7	• Repeat steps 3 to 6 on the ***Footer*** tab and the subsequent pages' ***Header*** tab. **Note:** All ***Header*** and ***Footer*** tabs contain the same options. You can have all information in either the header or footer or split information between the header and footer as required.

Step	Action
8	Click ***OK***.

How to add objects to the report

The table below describes how to add objects to the report. The various objects are described below this table.

Step	Action
1	• Click the appropriate icon in the ***Report items*** toolbar. *or* • Choose an object from the ***Insert*** menu. 
2	• Press and hold the left mouse button on the report page, and drag out a box to the size of the item you want to insert. **Note:** The mouse pointer shows a symbol for the type of item you have selected. • Release the mouse button. *Result*: A ***Setup*** dialog box opens. The dialog is specific to the type of item that you want to insert.
3	Select the desired options and click ***OK***. *Result*: The object is inserted onto the page.

Note: If you want to edit an object later, double-click the object box.

How to add free text

The table below describes how to add free text to the report:

Step	Action
1	• Click the ***Free Text*** icon. • Press and hold the left mouse button on the report page and drag out a box to the size of the text. Release the button. *Result*: The ***Setup Free Text*** dialog box opens.
2	• Type text in the edit field. • Select if the text is to start on a new page. • Select if the text box should be automatically sized. • Select if the text should appear in the same position on all pages, for example as header and footer text.
3	• Click the ***Font*** button to change the default font. *Result*: The ***Font*** dialog box opens. • Make the necessary changes and click ***OK*** to return.
4	Click ***OK***. *Result*: The text object is inserted onto the page.

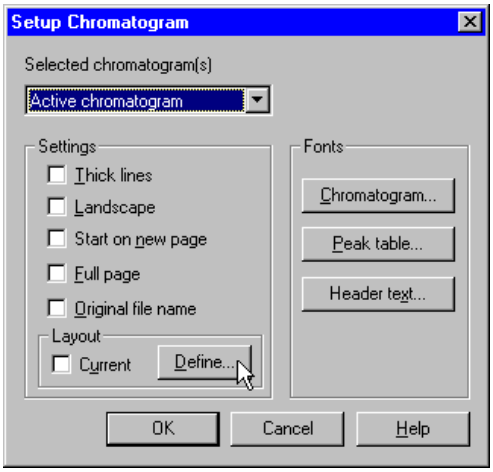
How to add a picture

The ***Picture*** dialog box is useful to insert logos, pictures or other image objects in the report. The table below describes how to add a picture object to the report:

Step	Action
1	• Press and hold the left mouse button on the report page and drag out a box to the size of the picture item. Release the mouse button. • Click the ***Picture*** icon. *Result*: The ***Picture*** dialog box opens.
2	• Click the ***Browse*** button to locate the desired picture file. • Select the picture file and click the ***Open*** button. **Note:** The file formats ***.bmp***, ***.emf***, ***.jpg*** and ***.tif*** can be used. *Result*: A preview of the selected picture is displayed.
3	Select the desired ***Settings*** and click ***OK***. *Result*: The picture is inserted onto the page.

How to add a chromatogram or peak table

The table below describes how to add a chromatogram to the report. The layout can also be defined to include a peak or pool table if desired.

Step	Action
1	• Click the ***Chromatogram*** icon. • Press and hold the left mouse button on the report page and drag out a box to the size of the chromatogram. Release the mouse button. *Result*: The ***Setup Chromatogram*** dialog box opens. 
2	Select which chromatogram(s) to insert from the ***Selected chromatogram(s)*** droplist: • ***Active chromatogram*** inserts the chromatogram that currently is active in the ***Evaluation*** module. • ***All chromatograms*** inserts all chromatograms that are open in the ***Evaluation*** module. • ***1, 2...etc.*** inserts the corresponding chromatogram.

Step	Action
3	• Select the desired ***Settings***. • If desired, change the ***Fonts***. **Note:** Separate fonts can be selected for the ***Chromatogram***, the ***Peak table*** and the ***Header text***.
4	• Click the ***Define*** button in the ***Layout*** field if you want to re-define the layout of the chromatogram. *Result*: The ***Report Chromatogram Layout*** dialog box opens. • Make the appropriate changes and click ***OK*** to return to the ***Setup Chromatogram*** dialog box. **Note:** The changes that you make will only affect the report and not the view of the chromatograms in the ***Evaluation*** module.
5	Click ***OK***. *Result*: The chromatogram is inserted onto the page.

Note: All curves can be de-selected in the ***Report Chromatogram Layout*** dialog box leaving only the selected peak table(s) in the report.

How to include a method

The table below describes how to include a method in the report:

Step	Action
1	• Click the ***Method*** icon. • Press and hold the left mouse button on the report page and drag out a box to the size of the item. Release the button. *Result*: The ***Setup Method*** dialog box opens.
2	Select the items to be included in the report: • ***Main Method*** is the method on which the run was based. • ***Blocks*** are the blocks that were used in the method.

Step	Action
3	• Select the appropriate ***Settings***. **Note:** ***Expand main*** displays the expanded method view. • If desired, change the ***Fonts***. • Click ***OK***. *Result*: The method object is inserted onto the page.

How to add documentation

The table below describes how to add documentation to the report:

Step	Action
1	• Click the ***Documentation*** icon. • Press and hold the left mouse button on the report page and drag out a box to the size of the item. Release the button. *Result*: The ***Setup Documentation*** dialog box opens.
2	Select the items to be included in the report: • ***Select All*** includes all items in the report. • ***Clear All*** removes all selections.
3	• If desired, change the ***Fonts***. • Select if the documentation should start on a new page. • If ***Select All***, ***Run summary*** or ***Logbook*** was selected, make the necessary changes to the ***Base*** and ***Logbook filter*** settings.
4	Click ***OK***. *Result*: The selected documentation items are inserted into the report.

How to add the Evaluation Log

The table below describes how to add the ***Evaluation Log*** to the report:

Step	Action
1	• Click the ***Evaluation Log*** icon. • Press and hold the left mouse button on the report page and drag out a box to the size of the item. Release the mouse button. *Result*: The ***Setup Evaluation Log*** dialog box opens.
2	• If desired, change the ***Fonts***. • Select if the ***Evaluation Log*** should start on a new page.
3	Click ***OK***. *Result*: The ***Evaluation Log*** is inserted into the report.

How to include Quantitate and Molecular Size data

The table below describes how to include ***Quantitate*** and ***Molecular Size*** data in the report.

Note: This option is only available if the ***Analysis*** module has been installed.

Step	Action
1	• Click the ***Quantitate and Mol Size*** icon. • Press and hold the left mouse button on the report page and drag out a box to the size of the item. Release the mouse button. *Result*: The ***Setup Quantitate*** dialog box opens.

Step	Action
2	• If desired, change the ***Fonts***. • The default option is that the ***Quantitate and Molecular Size*** data will start on a new page. • Click ***OK***. *Result*: The ***Quantitate and Molecular Size*** data is inserted into the report.

How to include Frac-950 data

The table below describes how to include ***Frac-950*** data in the report.

Note: This option is available only if a ***Frac-950*** has been installed and if the result file contains data from the ***Frac-950***.

Step	Action
1	• Click the ***Frac-950*** icon. • Press and hold the left mouse button on the report page and drag out a box to the size of the item. Release the mouse button. *Result*: The ***Setup Frac-950*** dialog box opens.
2	• If desired, change the ***Fonts***. • Select if the ***Frac-950*** data should start on a new page. • The ***Include rack layout*** option is selected by default. This will display the rack layout that was used in the run. • Click ***OK***. *Result*: The ***Frac-950*** data is inserted into the report.

How to move and resize objects freely

The table below describes how to select, move and resize objects freely:

If you want...	then...
to select a single object,	• click the ***Select*** icon, • click the object of interest.
to select several objects,	• click the ***Select*** icon, • press and hold the **Ctrl** key while you click the objects.
to move the selected object(s),	click on the objects, hold down the left mouse button and drag the object(s) to the new position.
to resize the selected object(s),	click one of the object border anchors, either in the corners or in the middle of a border, and drag the box to the new size. **Note:** Some ***Text*** objects cannot be resized.

Alignment toolbar icon functions

Objects can be placed in exact positions and sized in relation to other objects. The table below describes the function of the ***Alignment*** toolbar icons in the ***Report Editor***:

Toolbar icon	Function
	Align left Matches the left alignment of all selected objects to that of the highlighted object.
	Align right Matches the right alignment of all selected objects to that of the highlighted object.

Toolbar icon	Function
	Align top Matches the top alignment of all selected objects to that of the highlighted object.
	Align bottom Matches the bottom alignment of all selected objects to that of the highlighted object.
	Adjust to margins Stretches the selected object(s) to the left and right margins.
	Adjust to left margin Adjusts the selected object(s) to the left margin.
	Adjust to right margin Adjusts the selected object(s) to the right margin.
	Adjust to center Adjusts the selected object(s) to the center of the page.
	Make same size Adjusts the selected objects to the same size as the highlighted reference object.
	Make same width Adjusts the selected objects to the same width as the highlighted reference object.

Toolbar icon	Function
	Make same height Adjusts the selected objects to the same height as the highlighted reference object.

Note: The ***Make same size*** and ***Make same width*** functions can only be used to resize the width of chromatograms, free text and picture objects.

How to print the report

The table below describes how to print the report:

Step	Action
1	• Choose ***File:Print***. *or* • Click the ***Print*** icon. *Result*: The ***Print*** dialog box opens. **Note:** Printers are set up in the ***File*** menu of the ***UNICORN Manager***.
2	• Select the printing range. • Select the number of copies.
3	Click ***OK***.

Note: You can also print the report from the ***Generate Report*** dialog box.

How to save the report in PDF format

The table below describes how to save the finished report as a PDF file:

Step	Action
1	• Click the ***UNICORN Manager*** icon on the Windows taskbar. *Result*: The ***UNICORN Manager*** opens.
2	• Choose ***File:Printer Setup***. *Result*: The ***Print Setup*** dialog box opens.
3	• Select an Adobe Acrobat printer from the ***Printer Name*** list (e.g. Acrobat Distiller). • Click the ***Properties*** button and edit the document properties if needed. • Select the appropriate paper size and orientation. • Click ***OK***.
4	• Click the ***Evaluation*** icon on the Windows taskbar. *Result*: The ***Evaluation*** module opens
5	• Print the report as described in *"How to print the report"*. *Result*: The report is created as a PDF file and saved in the location specified in your Acrobat settings.

Note: You must have a full installation of Adobe Acrobat or a suitable printer driver to be able to do this.

How to save the report format

The table below describes how to save the finished report format:

Step	Action
1	• Choose ***File:Save***. *or* • Click the ***Save*** icon. *Result*: The ***Save Report Format*** dialog box opens.
2	• Type a name for the format. • Select if you want to save the format for global use. • Select if you want to save the format as default. **Note:** The name for the default format will automatically be changed to DEFAULT.
3	Click ***OK***.

10.6.2 How to create and print a standard report

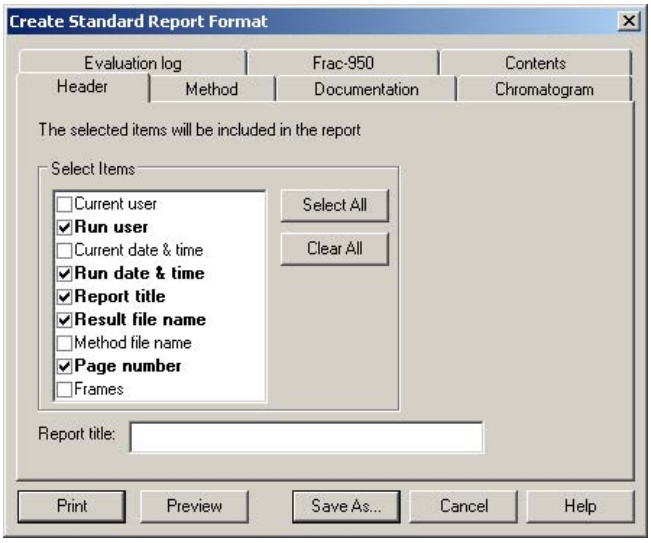
How to create a Standard report

You can only select a number of pre-formatted items when you create a ***Standard*** report format. If you want to edit the layout in detail you must create a ***Customized*** report format. See *Section 10.6.1 How to create and print a customized report, on page 303*.

The table below describes how to create and save a ***Standard*** report format:

Step	Action
1	Open a result file.
2	• Select ***File:Report***. *or* • Click the ***Report*** icon. *Result*: The ***Generate Report*** dialog box opens.
3	Click the ***New*** button. *Result*: The ***Create New Report Format*** dialog box opens.

Step	Action
4	• Select ***Standard format*** and click ***OK***. *Result*: The ***Create Standard Report Format*** dialog box opens. The illustration below shows the ***Create Standard Report Format*** dialog box with the ***Header*** tab selected:



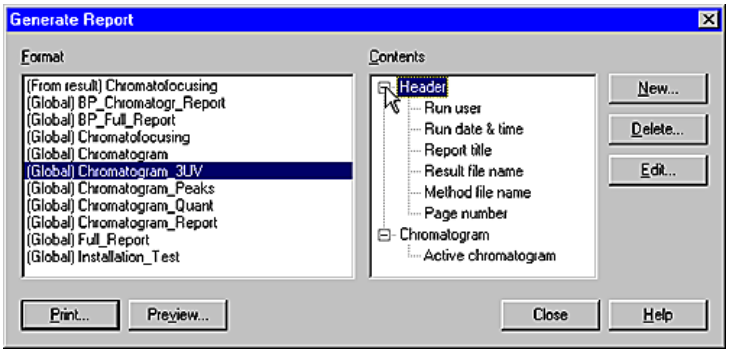
5	Click the appropriate tabs and select the check boxes for each item that you want to include in the report.
6	Click the ***Chromatogram*** tab and select the chromatogram(s) you want to include. • Select the ***Current*** option in the ***Layout*** field to apply the current layout in the ***Evaluation*** module. *or* • Click the ***Define*** button in the ***Layout*** field to open the ***Curve*** tab in the ***Report Chromatogram Layout***. - Select the curves that you want to include in the report and click ***OK***.

Step	Action
7	• Click the ***Contents*** tab to see a list of all the selected items. • Click the ***Preview*** button to see the entire report layout. • Click the ***Close*** button to return. • Click the ***Print*** button to print a test report.
8	• Click the ***Save As*** button. *Result*: The ***Save Report Format*** dialog box opens.
9	• Type a name in the ***Report format name*** text box. - Select the ***Save as global format*** check box to make the format available to other users. - Select the ***Save as default report format*** check box if desired (The format is saved as DEFAULT). - Click ***OK***. *Result*: The ***Generate Report*** dialog box opens again. The new report is saved and available in the ***Format*** list.
10	• Click the ***Close*** button *or* • Click the ***New*** button to create another ***Standard*** report.

How to print a standard report

The table below describes how to print a ***Standard*** report format in the ***Evaluation*** module.

Step	Action
1	Open a result file.

Step	Action
2	• Select ***File:Report***. • *or* • Click the ***Report*** icon. *Result*: The ***Generate Report*** dialog box opens. 
3	• Select a ***Standard*** report format. **Note:** The contents of a ***Standard*** report format is displayed in the ***Contents*** field. • Verify in the ***Contents*** field that the report format contains all the elements that you want to include. Click the ***Edit*** button to modify the report format if needed.
4	• Click the ***Print*** button. *Result*: The ***Print*** dialog box opens. • Choose what pages and how many copies to print. • Click ***OK***. **Note:** Printers are set up in the ***File*** menu of the ***UNICORN Manager***.

10.6.3 How to edit an existing report format

Introduction

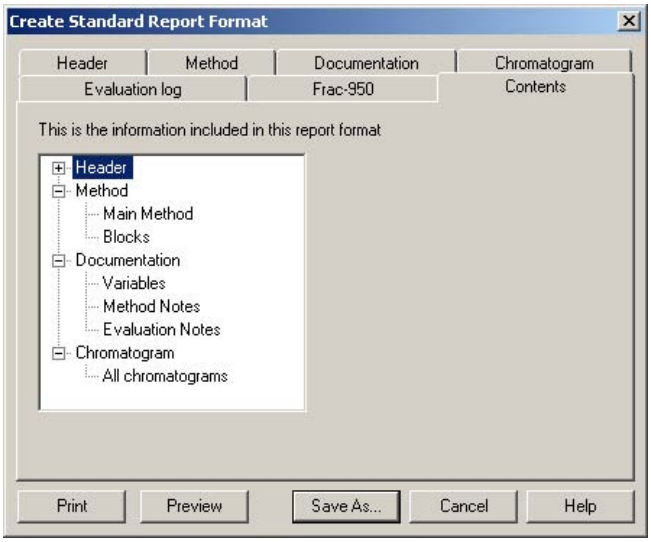
This section describes how to edit an existing report format.

How to edit a standard report

The table below describes how to edit a standard report format in the ***Evaluation*** module.

Step	Action
1	Open a result file.
2	• Select ***File:Report***. *or* • Click the ***Report*** icon. *Result*: The ***Generate Report*** dialog box opens.
3	• Select a ***Standard*** report format to edit. • Click the ***Edit*** button. *Result*: The ***Edit Report Format*** dialog box opens.
4	Select ***Standard format*** and click ***OK***. *Result*: The ***Edit Standard Report Format*** dialog box opens.
5	Click the appropriate tabs and select the check boxes for each item that you want to include in the report format. **Note:** See *Section 10.6.2 How to create and print a standard report, on page 320* for more information.

Step	Action
6	Click the ***Contents*** tab to see a list of all the selected items.



7	• Click the ***Save As*** button. *Result*: The ***Save Report Format*** dialog box opens.
8	• Type a name in the ***Report format name*** text box. - Select the ***Save as global format*** check box to make the format available to other users. - Select the ***Save as default report format*** check box if desired (The format is saved as DEFAULT). - Click ***OK***. *Result*: The ***Generate Report*** dialog box opens again. The new report format is saved and available in the ***Format*** list.
9	• Click the ***Close*** button. *or* • Click the ***Edit*** button to edit another report format.

How to edit a customized report

The table below describes how to edit a customized report format in the ***Evaluation*** module.

Step	Action
1	Open a result file.
2	• Select ***File:Report***. or • Click the ***Report*** icon. *Result*: The ***Generate Report*** dialog box opens.
3	• Select a ***Customized Report Format*** to edit. • Click the ***Edit*** button. *Result*: The report format opens in the ***Report Editor***.
4	• Double-click the report item you want to edit. • Make the desired changes in the dialog box. • Continue to edit all items until the format is complete. **Note:** See *Section 10.6.1 How to create and print a customized report, on page 303* for more information.
5	• Select ***File:Save As***. *Result*: The ***Save Report Format*** dialog box opens.
6	• Type a name in the ***Report format name*** text box. - Select the ***Save as global format*** check box to make the format available to other users. - Select the ***Save as default report format*** check box if desired (The format is saved as DEFAULT). - Click ***OK***. *Result*: The new report format is saved and available in the ***Format*** list.

10.7 Run documentation

Introduction

The full documentation for a run is stored in the result file. This section describes:

- some of the contents of the run documentation,
- how to view and print the run documentation,
- how to save the method from the run as a new method.

How to view and print the run documentation

The table below describes how to view and print the run documentation.

Step	Action
1	Open a result file.
2	• Choose ***View: Documentation*** in the ***Evaluation*** module. *or* • Click the view ***Documentation*** icon. *Result*: The ***Documentation*** dialog box opens. See further information about some of the tabs below.
3	Click the ***Print*** button. *Result*: The ***Print*** dialog box opens.
4	Select the documentation items you want to print and click ***OK***. *Result*: The documentation is printed on the default Windows printer.

The tabs of the Documentation dialog box

The table below describes the contents of some of the ***Run Documentation*** tabs.

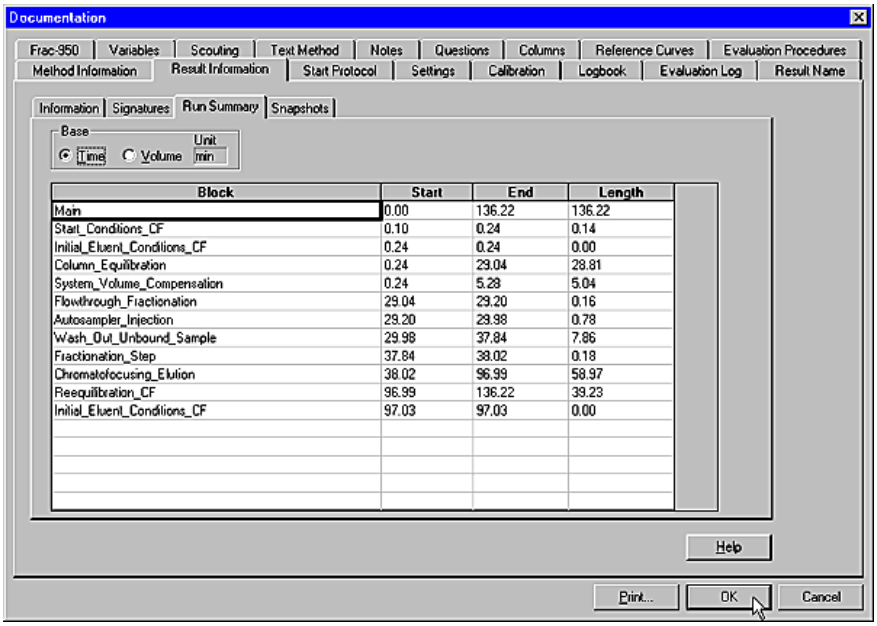
Documentation tab	Contents
Variables	The ***Variables*** tab lists the parameters that were used during the method run.
Scouting	The ***Scouting*** tab displays the whole scouting scheme, with the values for the current result file displayed in yellow cells.
Notes	The ***Notes*** tab displays the notes that you have made at various times during the method run. You are also able to type new comments on the ***Evaluation Notes*** sub-tab. *Note*: Click the ***Find*** button to search for a specific text string in the ***Notes***.
Calibration	The ***Calibration*** tab displays the system calibrations and when and by whom they were made.
Logbook	The ***Logbook*** tab displays what happened during a method run. You can view information concerning alarms, the method, manual changes during the run, errors, etc. *Note*: Click the ***Find*** button to search for a specific text string in the ***Logbook***.
Evaluation Log	The ***Evaluation Log*** lists all of the evaluation operations that you have performed for the result file during all sessions, including at the end of the method.
Method Information	The ***Method Information*** tab displays information about the method, such as the method name, the target system and the date of the last change. Information about the strategy includes name, date and size. There is also a sub-tab for ***Signatures***.
Frac-950	The ***Frac-950*** tab displays the setup parameters for the fraction collector provided it is included in the strategy.
Result Information	See "The Result Information tab" in this section.

The Result Information tab

The ***Result Information*** tab displays information about the result file, such as

- the result file name
- the system that was used
- the last date it was changed.

Information about the strategy includes name, date and size. The ***Run Summary*** sub-tab is a summary of the run expressed in volume or time per block. There is also a sub-tab for ***Signatures*** and a sub-tab where all ***Snapshots*** that have been taken during the run are displayed.



Save the method used for the run as a new method

You can save the method and the variables that were used for the run as a new method:

Step	Action
1	• Select the ***Text Method*** tab in the ***Documentation*** dialog box. • Click the ***Save as*** button. *Result*: The ***Save As*** dialog box opens.
2	• Select the appropriate destination folder. • Type a name in the ***Method name*** text box. • Select a system in the ***For System*** field. • Select ***Any*** in the ***Technique*** field. • Select a technique in the ***Technique*** field. • Click ***OK***. *Result*: The method is saved.

11 How to edit results

Introduction

This chapter describes

- how to edit the results that are presented in the ***Evaluation*** module
- how to import and compare runs
- how to import and export results.

For more information about how to view results, see chapter *Chapter 10 How to view results, on page 266*.

In this chapter

This chapter contains these sections:

Section	See page
11.1 How to reduce noise and remove ghost peaks	332
11.2 How to subtract a blank run curve	334
11.3 How to add curves	337
11.4 How to enter and edit text in the chromatogram	338
11.5 How to pool fractions	340
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11.1 How to reduce noise and remove ghost peaks

Introduction

Sometimes the chromatograms contain curves with a noisy baseline. The noise can be caused by several factors, for example a dirty flow cell, air bubbles, electrical noise, dirty buffers, etc. The amount of noise can usually be reduced by taking proper precautions, for example filtration of buffers and instrument maintenance.

You can also use the smoothing function to reduce or remove background noise from a selected curve. Smoothing is always a compromise between noise removal and preservation of peak shape.

How to smooth a curve

The table below describes how to select a smoothing function and smooth a curve:

Step	Action
1	Select ***Operations:Smooth***. *Result:* The ***Smooth*** dialog box is displayed.
2	Select the curve to be smoothed and its target destination.
3	Select the ***Filter type*** to be applied. The options are: • ***Moving average***. Use this if you have noise along most of the curve. It affects peak height but not retention. There is little effect on the peak area. • ***Autoregressive***. Use this if you have periodic noise along the whole curve. It affects peak height and retention, although this has little effect on the peak area. • ***Median***. Use this if there is only one or a few noise spikes, for example caused by air bubbles, or if the noise is confined to only a small part of the curve. It can flatten peaks and affect peaks areas slightly, but does not affect retention. • ***Savitzky-Golay***. Use this to calculate the smoothing and differentiation of data by a least squares technique.

Step	Action
4	Select an appropriate smoothing parameter value from ***Light*** to ***Hard*** for the selected filter in the ***Filter Parameters*** field. Use the slider, or insert a value manually in the text field. The smoothing effect increases with increasing parameter values. • Click ***OK***.

Tip: Start with a low parameter value, for example the default value, and increase it until the best result is achieved. A useful strategy is to increase the parameter value by the default value for each try.

Note: By default, smoothed curves are given the suffix ***SMTH***. The default curve name can be changed as needed.

11.2 How to subtract a blank run curve

Introduction

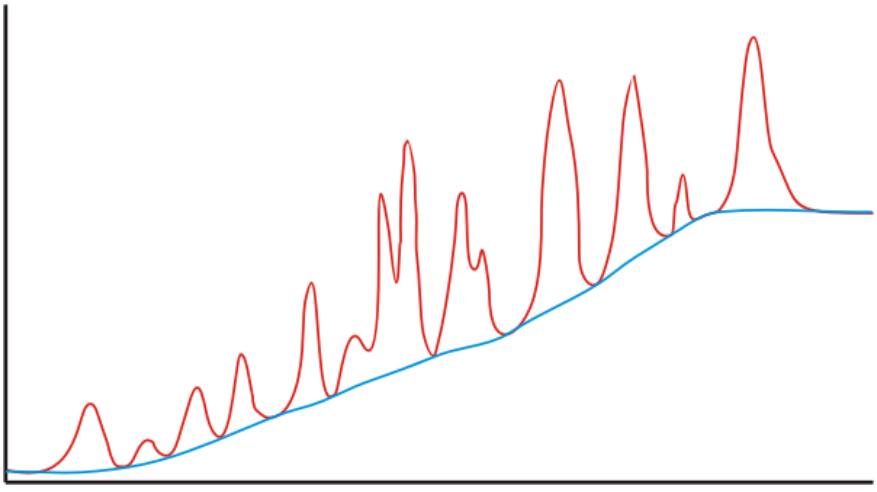
Subtracting a blank run curve is a frequently used function in presentations, especially if the curves have a drifting baseline or ghost peaks.

Ghost peaks

If the ghost peaks come from impurities in the eluents, all equilibration of the columns should be the same from method run to method run. If, for example, the equilibration volume with buffer A is larger before a blank run curve than before a separation, your ghost peaks might be higher in the blank run curve.

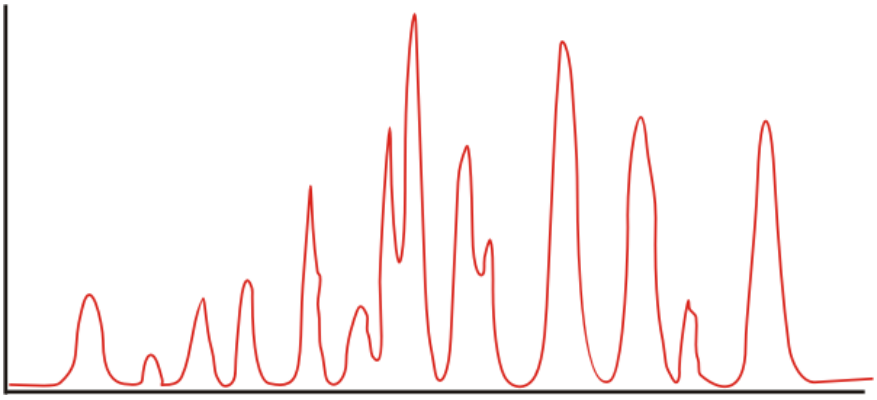
Example of a UV curve with baseline

The illustration below shows the UV curve with baseline prior to subtraction of the baseline:



Example of a UV curve after subtraction of the baseline

The illustration below shows the UV curve after subtraction of the baseline:



How to import a blank run curve

If a blank run curve was made, this might have been stored in another result file. If there is no blank run curve, you can create one with ***Integrate:Calculate baseline***. The table below describes how to import the blank run curve:

Step	Action
1	Ensure that the destination chromatogram has been opened and is the active window on the screen.
2	Choose ***File:Open:Curves***. *Result:* The ***Open Curves*** dialog box is displayed.
3	Double-click the result file that contains the blank run curve. *Result:* The curves in the first chromatogram are displayed.
4	Select the appropriate chromatogram in the ***Chromatogram list***. *Result:* The curves for that chromatogram are displayed on the ***Available*** list.
5	Select the curves that correspond to the blank run curve and click the ***Select*** button. *Result:* The selected curve is displayed on the ***Selected curves*** list.

Step	Action
6	If you want to remove a curve from the list, select it and click the ***Remove*** button.
7	Click ***OK*** to import the curve.

Note: For more detailed information on how to import curves, chromatograms and other results see *Section 11.8 How to import and compare different runs, on page 350*.

How to subtract a blank run curve

You can subtract the blank run curve or the baseline from the sample curve. The table below describes how to do this:

Step	Action
1	Select ***Operations:Subtract.*** *Result:* The ***Subtract*** dialog box is displayed.
2	Select the sample chromatogram and curve in the left field and the baseline or blank run curve to be subtracted in the middle field.
3	Click ***OK***.

Note: All resulting curves from the subtract operation receive the ***SUB*** suffix by default. The default curve name can be changed as needed.

11.3 How to add curves

Introduction

In some method runs, several sequential chromatograms might have been created. This can occur, for example, when the instruction ***New chromatogram*** has been used in the method, thus creating different chromatograms during the run.

In order to view and evaluate the resultant curve of all the chromatogram parts, the curves must be added together. Usually, you have a number of chromatograms within the same result file and you want to add the curves. In some circumstances, curves might need to be imported from other result files.

Instruction

The table below describes how to add curves:

Step	Action
1	Select and view the first chromatogram in the sequence.
2	Choose ***Operations:Add***. *Result:* The ***Add*** dialog box is displayed.
3	• Select the first curve in the desired sequence in the left field. • Select the second curve in the sequence in the middle field. • Click the ***OK*** button to add the two curves together in a new result curve.
4	• Open the ***Add*** dialog box again. • Select the result curve (***.ADD***) from the previous addition in the left field. • Select the next curve in the sequence in the middle field. • Click ***OK*** to add the two curves together in a new result curve.
5	Repeat steps 3 and 4 until all curves have been added together. The final curve should be the cumulative curve for the whole run.

Note: All curves created using the ***Add*** operation receive the ***ADD*** suffix by default. The default curve name can be changed as needed. The original curves are distinguished in the chromatogram by underlined curve names.

11.4 How to enter and edit text in the chromatogram

How to enter text

Text can be added to the chromatogram. The table below describes how to do this:

Step	Action
1	• Right-click the curves view of the chromatogram window and select ***Add text*** from the menu. *or* • Choose ***Edit:Text:Add***.
2	Click where you want to insert text in the chromatogram. *Result*: A text box opens.
3	Type the text.
4	Click outside the text box to set the text.

How to edit the text

The table below describes how to edit inserted text:

Step	Action
1	Choose ***Edit:Text:Edit***. *Result:* The ***Edit Texts*** tab of the ***Chromatogram Layout*** dialog box is displayed.
2	• Select the text that you want to edit and make the appropriate changes in the ***Selected text*** field. • Click the ***Change text*** button or the ***Delete text*** button. • Use the ***Font*** and ***Set Orientation*** buttons if needed, and make the desired changes in the resulting dialog boxes.
3	Click ***OK*** to apply the changes.

Shortcut option

You can also right-click outside the text box and select ***Edit Text Mode*** from the shortcut menu. This activates all the text boxes in the chromatogram. The list below describes how to edit the text:

- Click the text and type the new text.
- Click outside the text box to set the text.

11.5 How to pool fractions

Introduction

Fractions are collected sequentially during a separation. Each fraction contains a set volume of sample. This section describes how to pool the information on several fractions into a new curve.

How to view the contents of a fraction

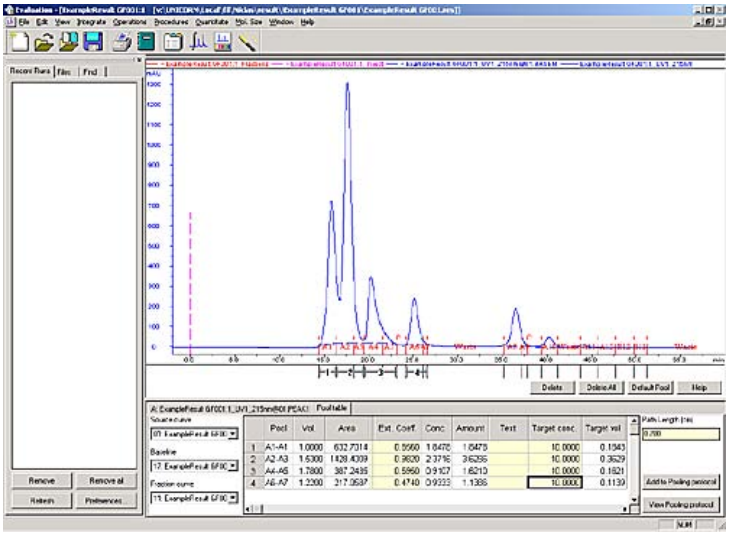
Each fraction is numbered according to its order in the sequence. The information is saved as a curve under the name ***Fractions***.

- Select this curve on the ***Curve*** tab in the ***Chromatogram Layout*** dialog box to display the contents of each fraction in relation to the information displayed on the UV detection curve.

How to pool fractions

The table below describes how to pool fractions.

Step	Action
1	• Choose ***Operations:Pool***. *Result*: UNICORN will automatically pool suitable fractions. The pooled fractions are listed in a table below the chromatogram and the pooled peaks are numbered sequentially in the chromatogram.



Note: Only adjacent fractions will be pooled. The fraction numbers for each pool are listed in the table as a range in retention order, e.g. A6-A7 etc.

Step	Action
2	The pooled fractions can be adjusted manually: **To include or exclude adjacent fractions in a pool** • Click the numbered marker under the pool and drag the sideline. **To add more pools** • Click between the droplines under a fraction to create a new pool, and drag the sidelines to include more adjacent fractions. **To delete pools** • Click the numbered marker to select the pool and click the ***Delete*** button. Click the ***Delete All*** button to clear all pools. **To restore the pools created by UNICORN** • Click the ***Default Pool*** button.
3	Other curves can be selected for the operation: • Select another source curve from the ***Source curve*** droplist and click the ***Default Pool*** button. *or* • Select another baseline curve from the ***Baseline*** droplist and click the ***Default Pool*** button. *or* • Select another fraction curve from the ***Fraction curve*** droplist and click the ***Default Pool*** button. *Result*: The pooled fractions in the list are replaced by the pooled fractions for the selected curve.

How to create a pool fraction curve

The pooled fractions can be stored as a new curve.

Note: You must store the pooled fractions as a new curve in order to be able to proceed with other operations using the pooled fractions.

Step	Action
1	Choose ***Operations:Create Pool Fraction*** curve. *Result*: The ***Create Pool Fraction Curve*** dialog box opens.

Step	Action
2	• Select a position where the curve will be stored from the ***Save curve in*** list. • If needed, type a new name in the ***Curve name*** text box. **Note:** The suggested curve name will have the default suffix ***POOL***.
3	Click the ***OK*** button. *Result*: The ***Pool Fraction*** curve is displayed in the chromatogram.

How to show only the pooled fractions

The active chromatogram will now show both the original and the pooled fraction curves. The table below describes how to show only the pooled fractions.

Step	Action
1	• Choose ***Edit:Chromatogram Layout***. *or* • Right-click in the chromatogram and choose ***Properties*** from the shortcut menu. *Result*: The ***Chromatogram Layout*** dialog box opens.
2	• Select the ***Curve*** tab. • De-select the check box for the original fraction curve (remove the check mark). *Result*: The original fraction curve is de-selected and is not displayed.

How to calculate concentration and amount in the pools

Protein concentrations

The protein concentration in the fractions are calculated using the following formula:

Concentration [mg/ml] = A / (d * 1000 *Ext.Coeff.)

A = Average fraction absorbance = ***Area / Volume [mAu]***.

d = UV-cell path length [cm]

Ext.Coeff. = Protein coefficient at used wavelength. [l g^{-1} cm^{-1}]

Protein amounts

The total amount of protein found in the pool fraction is calculated using the following formula:

Amount [mg] = Concentration [mg/ml] * pooled fraction volume [ml]

How to calculate the concentrations and amounts:

- Type the UV path length expressed in centimeters in the ***Path Length*** text box.
- Type the extiction coefficient in the ***Ext.Coeff.*** table cell for each pool.

Result: The sample concentration and amount for each pool is calculated in the corresponding table cell.

How to determine a pool target volume

The ***Target conc.*** and ***Target vol.*** cells are used to calculate the pool volume at a specific concentration level. The result can then be used to determine if the pool needs to be concentrated further or diluted.

- Type the desired concentration level (mg/ml) in the ***Target conc.*** table cell.

Result: The corresponding target volume is calculated in the ***Target vol***. table cell using the following formula:

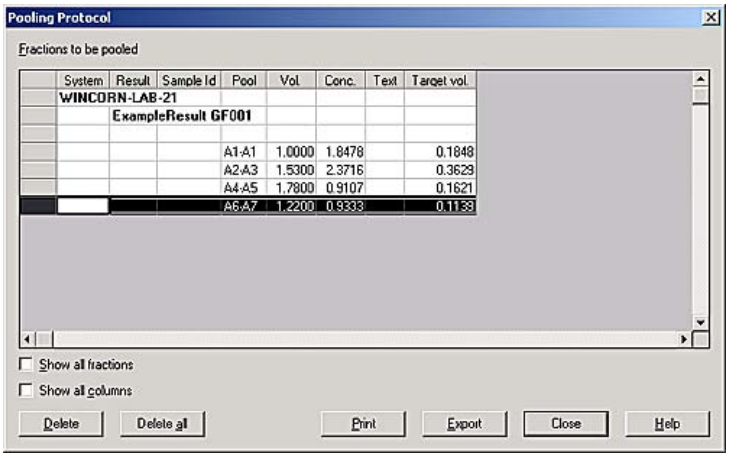
Target vol. = Conc. * (Vol./Target conc.)

How to use the Pooling Protocol

A protocol of the pooled fractions can be printed for use when handling the samples. The table below describes how to add pools to the ***Pooling Protocol*** and send the list to a printer or export the list to a file.

Step	Action
1	• Open a result file in the ***Evaluation*** module. • Pool fractions as described in *"How to pool fractions"* above. • Click the ***Add to Pooling Protocol*** button. *Result*: The pooled fractions from the active result file is added to the ***Pooling Protocol***.

Step	Action
2	• Repeat step 1 to add pooled fractions from other result files. **Note:** You will be asked to save the current file when you open the next. The pool table will not be saved.
3	• Click the ***View Pooling Protocol*** button. *Result*: The ***Pooling Protocol*** dialog box opens.



Step	Action
4	• Click the ***Show all fractions*** checkbox to display the individual fractions instead of fraction ranges for the pools. • Click the ***Show all columns*** checkbox to display all the information columns from the ***Pool table***. **Possible actions in the Pooling Protocol** To delete a single pool... • select a pool and click the ***Delete*** button To clear the whole protocol... • click the ***Delete all*** button. To print the protocol on the default Windows printer... • click the ***Print*** button to print the protocol on the default Windows printer. To export the protocol... • click the ***Export*** button to save the protocol in one of the following formats: - text (.txt) - Excel (.xls) - HTML (.htm) - XML (.xml) **Note:** The protocol is automatically saved for the user. The pooling protocol will be available again when the user starts UNICORN the next time.
5	• Click the ***Close*** button to close the ***Pooling Protocol*** dialog box. *Result*: If the protocol was exported or only edited, the dialog box will close. If the protocol was printed, a dialog box will open asking if you want to delete the list and start a new.

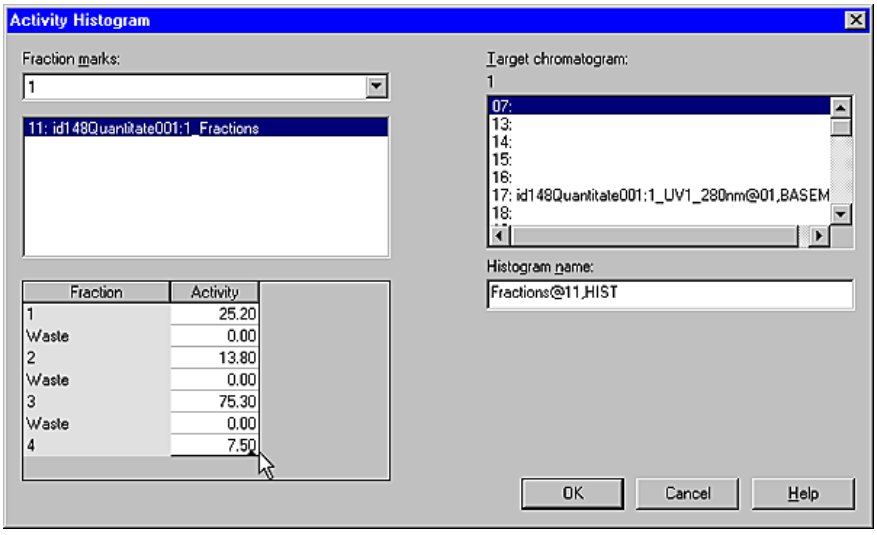
11.6 How to match protein activity to a curve

Introduction

You can compare data from the results of protein activity assays, such as ELISA, with the data contained in the UV curve. The activity curve and the UV curve can be compared in a combined presentation.

The Activity Histogram dialog box

The illustration below shows the ***Activity Histogram*** dialog box:



How to enter protein activity values for comparison

The table below describes how to enter the values from a protein activity assay in a comparison histogram:

Step	Action
1	Choose ***Operations:Activity Histogram***. *Result*: The ***Activity Histogram*** dialog box opens.
2	By default, the fraction curve for the specific chromatogram is selected. • If necessary, change the source and target chromatograms.
3	All the component fractions of the fraction curve are listed in the ***Fraction/Activity*** field. • Type an activity value for each fraction in the ***Activity*** column.
4	Click ***OK***.

11.7 How to rename chromatograms, curves and peak tables

Instruction

The table below describes how to rename chromatograms, curves or peak tables in the ***Evaluation*** module:

Step	Action
1	Choose ***Edit:Rename*** and the relevant option ***Chromatogram***, ***Curve*** or ***Peak Table***. *Result*: The ***Rename*** dialog box opens.
2	Select the appropriate object.
3	Type a new name in the ***Name*** field.
4	Click ***OK***.

Note: The original raw data curves cannot be renamed. They will not be listed as options in the dialog box.

11.8 How to import and compare different runs

Introduction

This section describes

- how to make comparisons between curves or chromatograms from different runs
- how to present curves or chromatograms from different runs.
- how to compare curve parameters among curves from different runs
- how to view several chromatograms at the same time
- how to overlay curves from different runs in one chromatogram
- how to stack curves from different runs in one chromatogram
- how to stretch curves to make comparisons easier
- how to create mirror images

In this section

This section contains these sub-sections:

Section	See page
11.8.1 How to use the Multifile Peak Compare wizard	351
11.8.2 How to import and compare chromatograms	367
11.8.3 How to import and compare curves	371
11.8.4 How to stack and stretch curves	380
11.8.5 How to produce a mirror image	385

11.8.1 How to use the Multifile Peak Compare wizard

Introduction

This section describes how to use the ***Multifile Peak Compare*** wizard to make comparisons between different results, for example, by comparing area, retention etc. The difference can be presented graphically or in a spreadsheet.

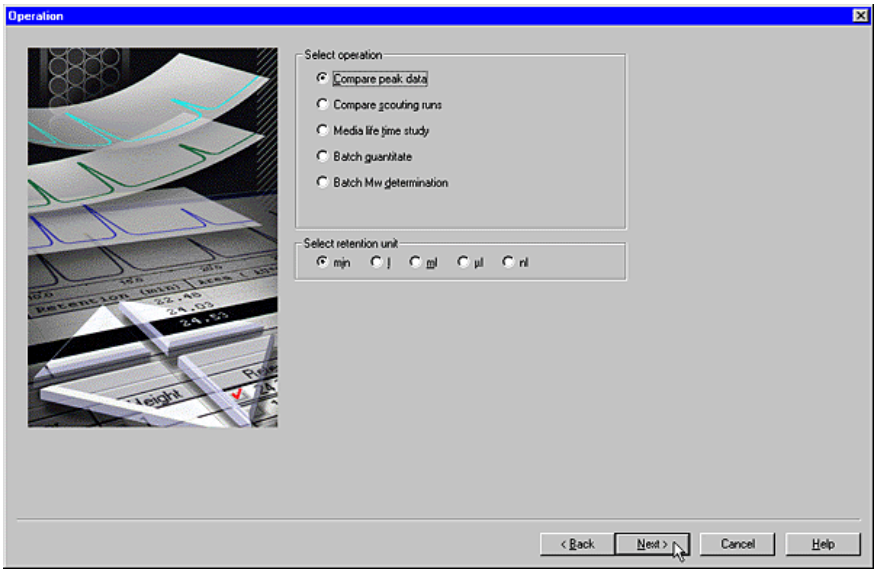
Step 1: How to select the Operation

The table below describes how to select the operation:

Step	Action
1	In the ***Evaluation*** module, • choose ***File:Multifile Peak Compare:Start Wizard*** *or* • click the ***Multifile Peak Compare*** toolbar icon: *Result*: The ***Multifile Peak Compare*** wizard entry dialog box is displayed.
2	Click the ***Next*** button to display the ***Operation*** dialog box.
3	Select • one of the available operations (see descriptions of the operations below this table) • a retention unit. If you select ***Batch quantitate***: • Select a quantitation table in the ***Select quantitation table*** field. If you select ***Batch Mw determination***: • Select a molecular size table in the ***Select mol. size table*** field. Click the ***Next*** button to proceed to the ***Data Selection*** dialog box.

The Operation dialog box

The illustration below displays the ***Operation*** dialog box:



The operation options

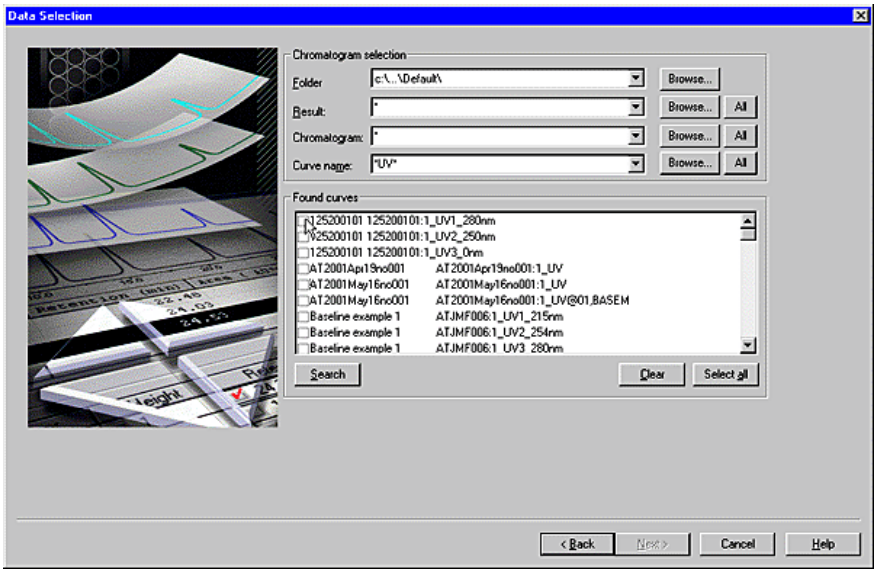
The table below is a brief description of the operation options:

Operation	Description
Compare peak data	This option is used to compare different results.
Compare scouting runs	This option is used to compare the results from scouting runs. The scouting variables can be displayed.
Media life time study	This option features different default values than the ***Compare peak data*** option, specially selected to measure changes in the column media.
Batch quantitate	This option is used to run several quantitations. This is an alternative to ***Quantitate:Calculate Amount and Conc.*** which is used to quantitate single results. A quantitation table must be created before this option can be used. This option is available only if the ***Analysis*** module has been installed.

Operation	Description
Batch Mw determination	This option is used to batch run molecular size calculations. This is an alternative to ***Mol. Size:Calculate Mol.Size***, which is used for single calculations. A molecular size table must be created before this option can be used. This option is available only if the ***Analysis*** module has been installed.

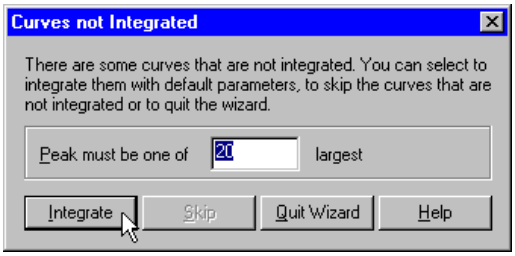
The Data Selection dialog box

The illustration below shows the ***Data Selection*** dialog box.



Step 2: How to select data to compare

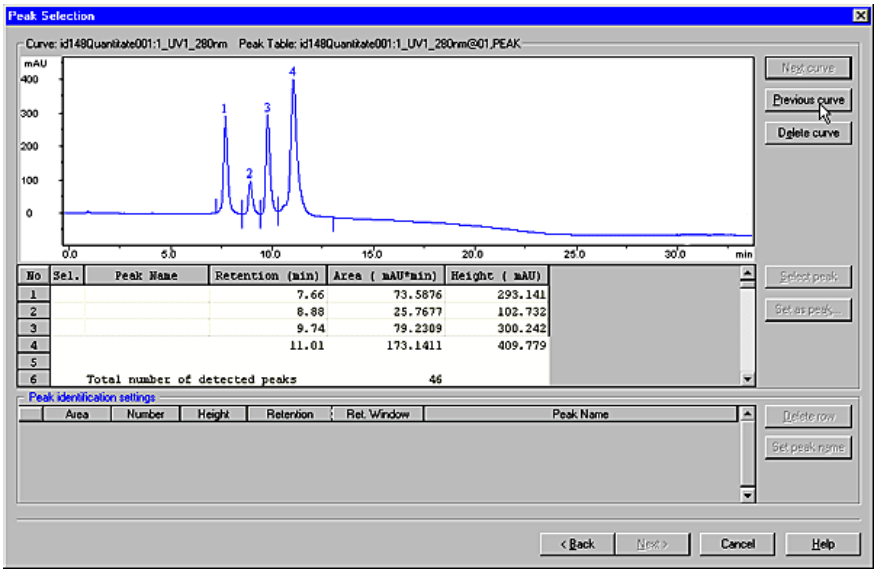
The table below describes how to select data to compare:

Step	Action
1	• Use the drop-down lists and ***Browse*** buttons in the ***Chromatogram selection*** field to specify the result files, chromatograms and curves for comparison. • Click the ***All*** button if you want to select all available results, chromatograms or curves.
2	• Click the ***Search*** button in the ***Found curves*** field. *Result*: A list of all curves that matched the search criteria is displayed in the ***Found curves*** field.
3	• Select the check boxes (or click the ***Select All*** button) of the desired curves within the ***Found curves*** field. • Click the ***Next*** button to proceed to the ***Peak Data Selection*** dialog box.
4	• If all the chosen curves have been integrated, go to "Step 3: How to select the peaks" in this section. • If any of the chosen curves have *not* been integrated, the ***Curves not Integrated*** dialog box is first displayed:  • If desired, change the default value for the peak number selection filter. • Click the ***Integrate*** button. *Result*: The ***Peak Selection*** dialog box is displayed. *Note*: If the results from the automatic peak integration is not satisfactory you must cancel the wizard and perform the integration manually. See *Section 12.1.2 How to perform a peak integration, on page 403*.

Curves not Integrated
There are some curves that are not integrated. You can select to integrate them with default parameters, to skip the curves that are not integrated or to quit the wizard.
Peak must be one of
20
largest
Integrate
Skip
Quit Wizard
Help

The Peak Selection dialog box

The illustration below displays the ***Peak Selection*** dialog box:



Dialog box description

The dialog box displays the following properties for the first of the chosen curves:

- The integrated peak and the associated peak table
- The ***Peak identification settings*** table. Its purpose is to identify the peak parameter to be used in the comparison.

How to adjust improper peak integrations

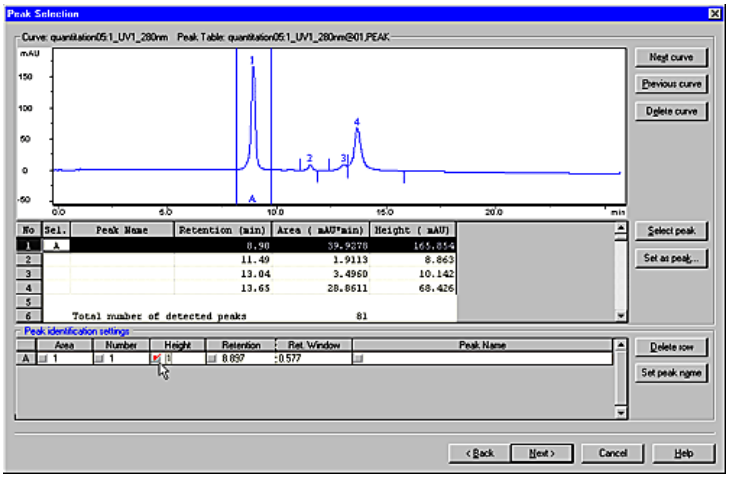
The table below describes what to do if the peaks in the curve window do not appear to be integrated properly (for example if ghost peaks are labelled).

Step	Action
1	Click the ***Cancel*** button to quit the wizard.
2	Perform a peak integration (see *Section 12.1.2 How to perform a peak integration, on page 403*) and verify that the resulting curve is properly integrated.
3	Repeat the ***Multifile Peak Compare*** wizard operation.

Step 3: How to select the peaks

The table below describes how select peaks in the ***Peak Selection*** dialog box:

Step	Action
1	Choose a curve in the curve window: • Double-click the peak, or click the peak once and then click the ***Select peak*** button. *Result*: The peak is assigned a letter (A, B, C....) and the peak parameters are displayed in the ***Peak identification settings*** table.
2	Set the desired peak identification criterion: • Click the desired parameter value in the ***Peak identification settings*** table. *Example*: If you have selected the highest peak in the curve and want to compare the highest peak among all curves, select the ***Height*** check box. In the illustration below, the initial (A) peak and the ***Height*** check box have been selected:



Step	Action
3	If desired, you can assign a name to a chosen peak: • Click the name of the row, for example ***A***. • Click the ***Set peak name*** button. • Type a new name and click ***OK***. *Note*: This can be useful when you compare multiple peak parameters and you wish to have peak names other than "Peak A", "Peak B", etc. to simplify peak identification and clarity f.ex. when comparing peak data between batch quantitated results.
4	Repeat steps 1-3 for other desired peaks in the current curve.
5	Use the ***Next curve*** and ***Previous curve*** buttons to navigate forward and backward among your selected curves and manually check the selections made by the software if necessary.
6	**Other possible actions you can perform** • If the current curve does not prove useful for your comparison, click the ***Delete curve*** button to delete it from the comparison. • Click the ***Back*** button to navigate back to the ***Data Selection*** dialog box and add new curves to your comparison. See also How to change the peak identification below.
7	When all peak selections and identification settings are complete, click the ***Next*** button to proceed to the ***Peak Data Selection*** dialog box.

Note: Click and drag in the curve window to zoom into selected peaks to simplify accurate peak identification. Right-click and click the ***Reset Zoom*** button to reset the zoom to the full view.

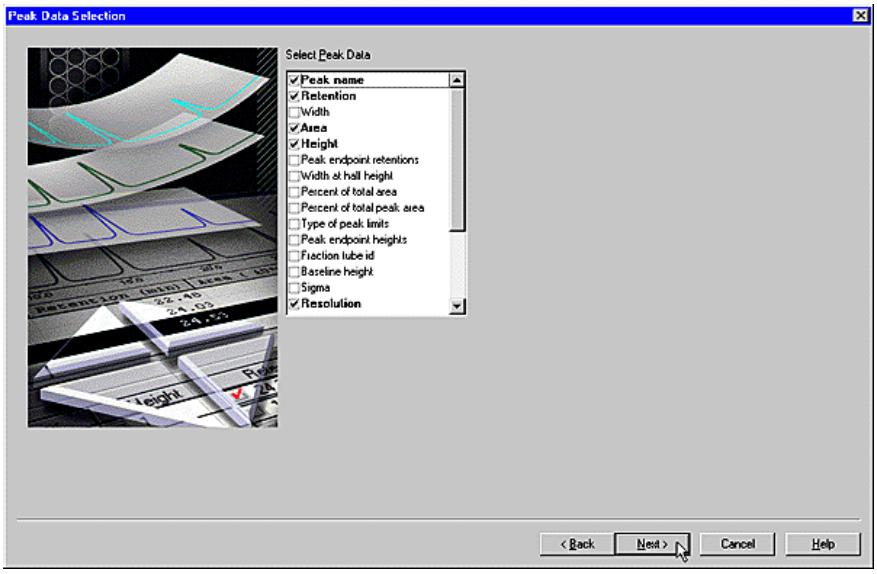
How to change the peak identification

In the ***Peak identification settings table***, each column identifies a peak parameter to be compared among all peaks. If UNICORN has identified other peaks than the intended ones, you can change the peak identification manually. The table below describes how to change the identification:

If you want to...	then...
remove a peak identification	• click the desired peak in the curves window • click the ***Set as peak*** button • choose ***None*** in the ***Set As Peak*** dialog box • click ***OK***.
replace or add a peak identification	• click a peak in the curves window • click the ***Set as peak*** button • choose a letter in the ***Set As Peak*** dialog box • click ***OK***.
remove a row from the table	• select the row • click the ***Delete row*** button. *Note*: If you click ***Delete row*** without first selecting a row, the first row (A) is deleted by default.

Step 4: How to select the Peak Data

The illustration below displays the ***Peak Data Selection*** dialog box:

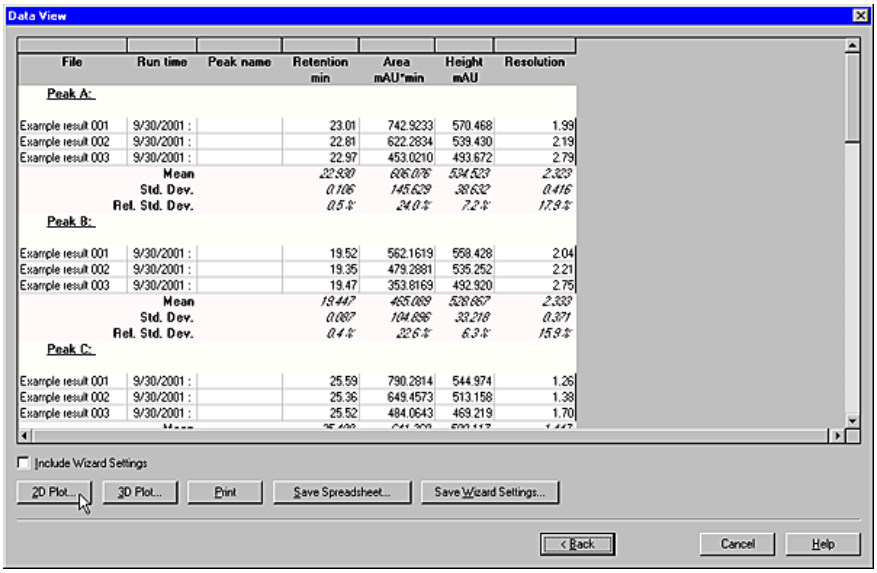


The table below describes how to select the peak data:

Step	Action
1	• In the ***Select Peak Data*** list, select the peak characteristics on the list that you want to include in your comparisons. • If available, select the appropriate ***Scouting*** variables.
2	• Click the ***Next*** button and proceed to step 5, How to use the ***Data View*** dialog box below. *Note*: If ***Media life time study*** was chosen in the ***Operation*** dialog box when the wizard was started, ***2D Plot*** is selected in the ***Data View*** dialog box.

Step 5: How to use the Data View dialog box

The ***Data View*** dialog box presents a comparison of the chosen data for the designated peak comparisons. The illustration below shows the dialog box:

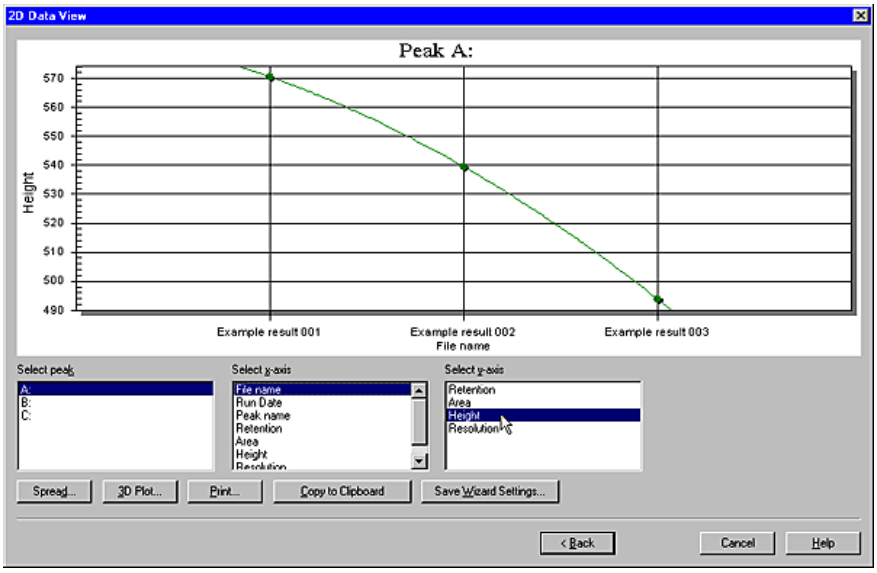


The table below describes how to use the command buttons of the dialog box:

Command button	Function
2D Plot	Displays the data in 2-dimensional plot. See "How to use the 2D Data View dialog box" below.
3D Plot	Displays the data in 3-dimensional plot. See "How to use the 3D Data View dialog box" below..
Print	Prints the spreadsheet.
Save Spreadsheet	Allows you to save the data in different formats: • Excel (.xls) • Tabbed text (.txt) • FarPoint spread (.ss3)
Save Wizard Settings	See "How to save the Wizard Settings" below.
Cancel	Ends the ***Multifile Peak Compare*** wizard.

How to use the 2D Data View

The ***2D Data View*** dialog box presents a two-dimensional plot of a selected peak. See also "How to use the 2D Data View shortcut menu" below. The illustration below shows the dialog box:



The list boxes

Use the list boxes to select which peak to plot and the units of the x- and y-axes.

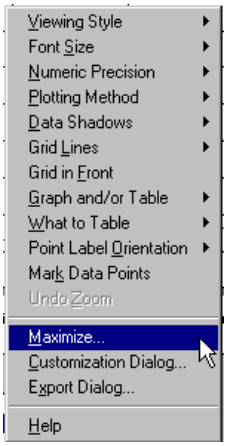
The command buttons

The table below describes how to use the command buttons of the dialog box:

Command button	Description
Spread	Returns to the ***Data View*** dialog box.
3D Plot	Displays the data in 3-dimensional plot. See "How to use the 3D Data View dialog box" below.
Print	Prints the spreadsheet.
Copy to Clipboard	Stores a figure for transfer to an external program.
Save Wizard Settings	See "How to save the Wizard Settings" below.
Cancel	Ends the ***Multifile Peak Compare*** wizard.

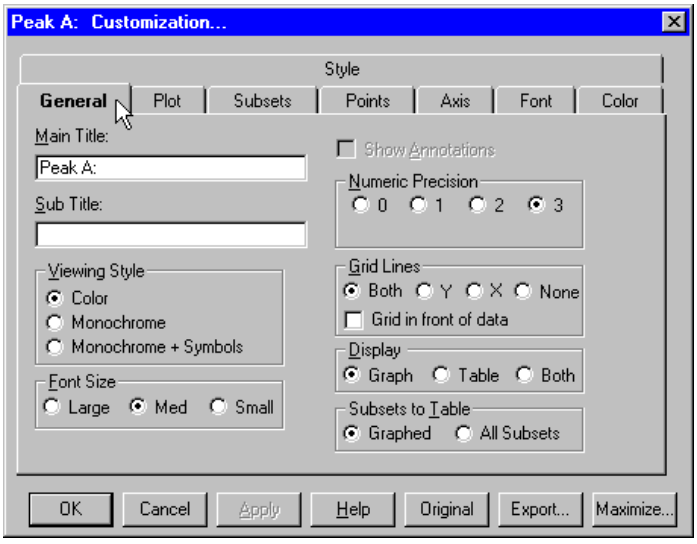
How to use the 2D Data View shortcut menu

Click the right mouse button in the plot area of the ***2D Data View*** dialog box to open the shortcut menu. See illustration below:



A wide array of plot presentation options can be found on the shortcut menu. Two of them are described below:

- Select ***Customization Dialog*** to open a dialog box which allows further customization of the graph:

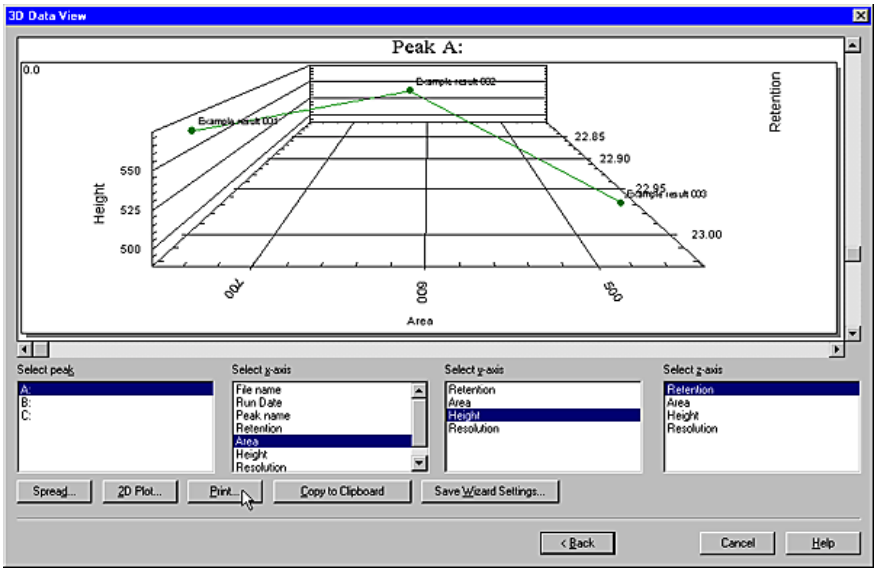


- Select ***Export Dialog*** to export the view.

Note: You can also click the ***Export*** button from the ***Customization*** dialog box.

How to use the 3D Data View dialog box

The ***3D Data View*** dialog box presents a three-dimensional plot of a selected peak. See also "How to use the 3D Data View shortcut menu" below. The illustration below shows the dialog box:



The list boxes

Use the list boxes to select which peak to plot and the units of the x-, y- and z-axes.

The command buttons

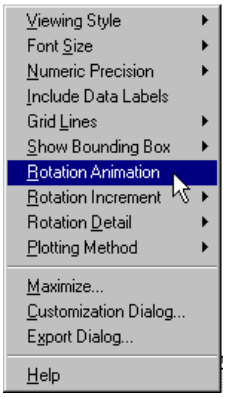
The table below describes how to use the command buttons of the dialog box:

Command button	Function
Spread	Returns to the ***Data View*** dialog box.
2D Plot	Displays the data in 2-dimensional plot. See "How to use the 2D Data View dialog box" above.
Print	Prints the spreadsheet.
Copy to Clipboard	Stores a figure for transfer to an external program.

Command button	Function
Save Wizard Settings	See "How to save the Wizard Settings" below.
Cancel	Ends the ***Multifile Peak Compare*** wizard.

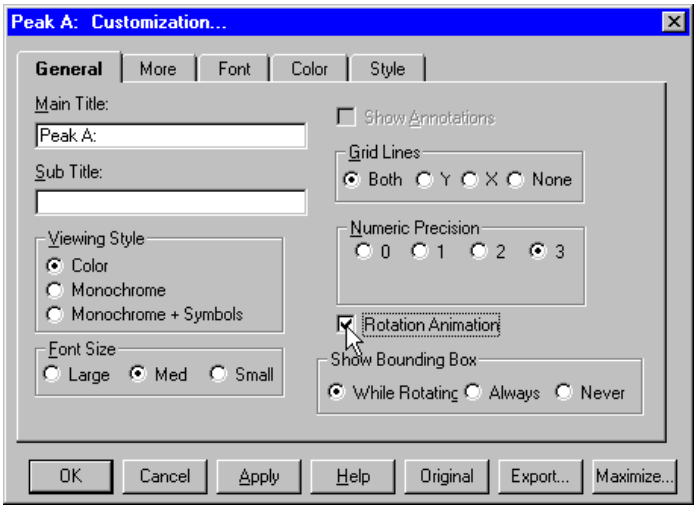
How to use the 3D Data View shortcut menu

Click the right mouse button in the plot area of the ***3D Data View*** dialog box to open the shortcut menu. See illustration below:



The ***3D Data View*** shortcut menu differs some from the ***2D Data View*** shortcut menu and allows the figure to be viewed by animated rotation. The shortcut menu displays different plot presentation options.

- Select ***Customization Dialog*** to open a dialog box that allows further customization of the graph:



- Select ***Export Dialog*** to export the view.

Note: You can also click the ***Export*** button from the ***Customization*** dialog box.

How to save the Wizard Settings

The wizard settings can be saved from either of these dialog boxes:

- The ***Data View*** dialog box
- The ***2D Data View*** dialog box
- The ***3D Data View*** dialog box

The table below describes how to save the wizard settings:

Step	Action
1	• Click the ***Save Wizard Settings*** button. *Result*: The ***Save Wizard Settings*** dialog box opens.
2	Type a name in the ***Wizard settings name*** field.

Step	Action
3	• If the settings are to be used by all users on the system, select the ***Global wizard settings*** check box. • Click ***OK***. • Click ***Cancel*** to close the wizard. *Note*: The ***Global wizard settings*** check box can also be used to toggle between lists of stored global and stored user settings.

How to open the saved wizard settings

The table below describes how to open the saved wizard settings:

Step	Action
1	• Choose the ***File:Multifile Peak Compare:Start Wizard With Settings*** menu item. *Result*: The ***Select Wizard Settings*** dialog box opens.
2	• Select the desired saved settings from the list. • Click ***OK***. *Result*: The ***Multifile Peak Compare*** wizard opens with the saved settings. *Note*: The ***Global wizard settings*** check box is used to toggle between lists of stored global and stored user settings.

11.8.2 How to import and compare chromatograms

Introduction

This section describes

- how to import chromatograms from other result files,
- how to compare with chromatograms in an already opened result file.

Commands to use

Two commands in the ***Evaluation*** module can be used to import chromatograms from result files into an already opened result file:

- ***File:Open to compare***

  This is the preferred option when you search for many chromatograms in a *specific* folder based on defined selection criteria. See "How to import chromatograms with the command ***File:Open to compare***" below.

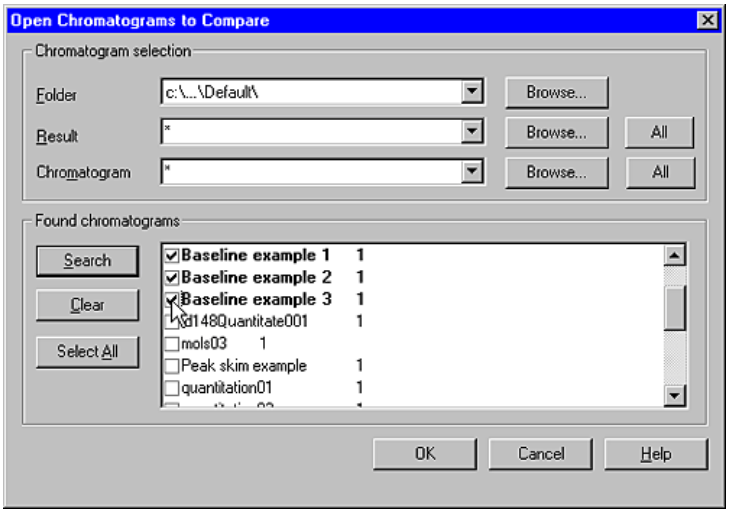
- ***File:Open***

  This is the preferred option to import any individual chromatograms from result files in *different* folders. See "How to import chromatograms with the command ***File:Open***" below.

How to import chromatograms with the command File:Open to compare

The table below describes how to import chromatograms with the ***File:Open to compare*** command. The search is performed at specific locations or with specific search criteria. This method is useful if you, for example, want to import chromatograms from all files of a scouting folder.

Step	Action
1	Choose ***File:Open to compare:Chromatograms*** in the ***Evaluation*** module. *Result*: The ***Open Chromatogram to Compare*** dialog box is displayed.



2	Click the ***Search*** button in the ***Found chromatograms*** field and a list of chromatograms will be displayed based on the designated search criteria. A new search can be performed with new search criteria without erasing the first found chromatograms from the list.
3	Select the chromatograms that you want to import. If you click the ***Select All*** button, all the displayed chromatograms will be imported. If you want to clear the list of displayed chromatograms, click the ***Clear*** button. **Note:** If the names of the imported chromatograms already are used they will be sequentially numbered for identification purposes. Up to 10 chromatograms can be made available at the same time in the ***Evaluation*** workspace.

Step	Action
4	Click ***OK***. *Result*: All the selected chromatograms are shown in the ***Evaluation*** workspace.

How to import chromatograms with the command File:Open

The table below describes how to import chromatograms one by one, using the command ***File:Open***:

Step	Action
1	Choose ***File:Open:Chromatogram*** in the ***Evaluation*** module. *Result*: The ***Open Chromatograms*** dialog box is displayed.
2	Double-click a result file to select it. *Result*: All the chromatograms contained in the result file will be displayed in the ***Available*** field.
3	Select the chromatogram(s) of interest and click the ***Select*** button. *Result*: Selected chromatograms are added to the ***Selected chromatograms*** list. **Note:** Chromatograms can be deselected with the ***Remove*** button.
4	Repeat steps 2-3 if you want to import chromatograms from other result files.
5	Click ***OK***. **Note:** If the names of the imported chromatograms already are used they will be sequentially numbered for identification purposes. Up to 10 chromatograms can be made available at the same time in the ***Evaluation*** workspace.

How to display and compare the imported chromatograms

The table below describes how to simultaneously display and compare the imported chromatograms:

Step	Action
1	In the ***Evaluation*** module, select • ***Window:Tile*** to display the chromatograms side by side. *or* • ***Window:Cascade*** to display the chromatograms in layers. **Note:** Chromatogram windows can be individually sized and the presentation of the curves changed.
2	**Display all chromatograms on the same scale** • Open the ***Chromatogram Layout*** dialog box for any chromatogram • Make the changes to the chromatogram axes. • Select the ***Apply to all chromatograms*** option.

Note: Imported chromatograms cannot be shown with column volume as the X-axis base.

11.8.3 How to import and compare curves

Introduction

This section describes how to import or copy curves from different runs into one chromatogram for comparison.

Commands to use

Two commands can be used to import curves from result files into one chromatogram:

- ***File:Open to compare***

  This is the preferred option if you want to automatically search result files that are stored in the same folder to locate all curves of a specified type, for example, all UV curves. This is especially useful for comparison of curves from scouting runs. Moreover, the imported curves can be automatically overlaid, stacked or presented as mirror images. See *"How to use File:Open to compare"* below.

- ***File:Open:Curves***

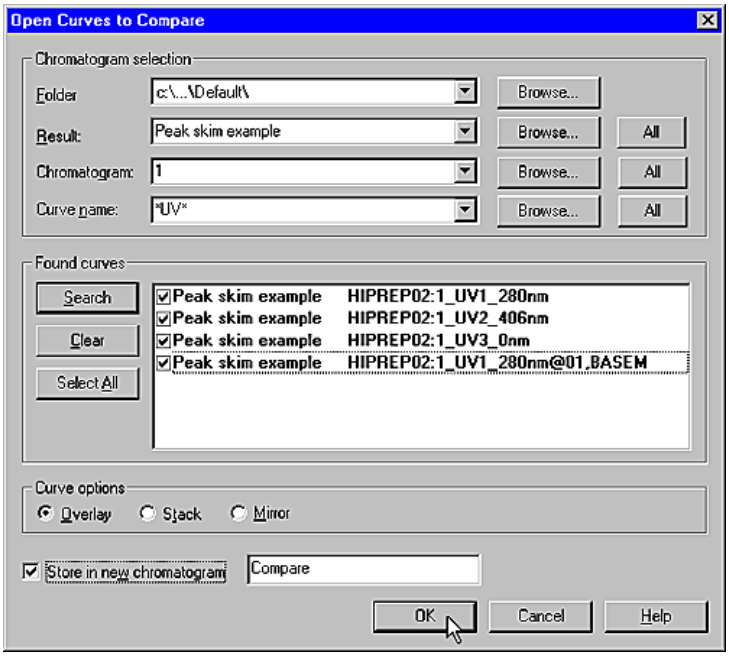
  This is the preferred option to import individual curves. See *"How to use File:Open:Curves"* below.

Note: Original curves are underlined in the chromatogram, imported and created curves are not underlined.

How to use File:Open to compare

The table below describes how to import curves to a chromatogram with the command ***File:Open to compare***:

Step	Action
1	In the ***Evaluation*** module, • choose ***File:Open to compare:Curves*** *or* • click the ***Open curves to compare*** toolbar button. *Result*: The ***Open Curves to Compare*** dialog box opens.

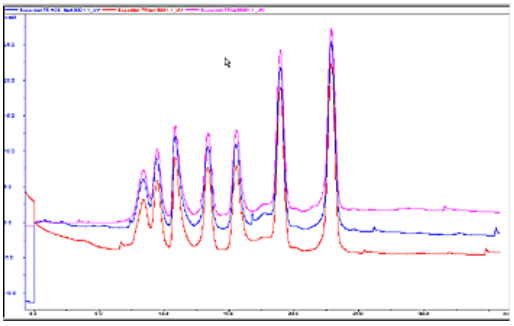


2	• Select the desired search criteria in the ***Folder***, ***Result***, ***Chromatogram*** and ***Curve name*** droplists of the ***Chromatogram selection*** section. • Click ***Search*** and a list of found curves will be displayed based on the selected search criteria. **Note:** A new search can be performed with new search criteria without erasing curves located in the previous search.

Step	Action
3	Select the check boxes for the curves that you want to import. Click the ***Select All*** button if you want to import all the curves. If you select the ***Store in new chromatogram*** option, the curves will be imported into a new chromatogram. This is recommended to keep the source chromatogram free of too many additional curves.

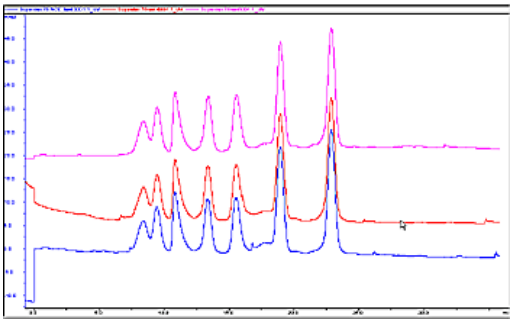
Step	Action
4	Select how to display the imported curves in the ***Curve options*** field and click ***OK***. See the options below:

Overlay



The curves are presented overlaid on one another.

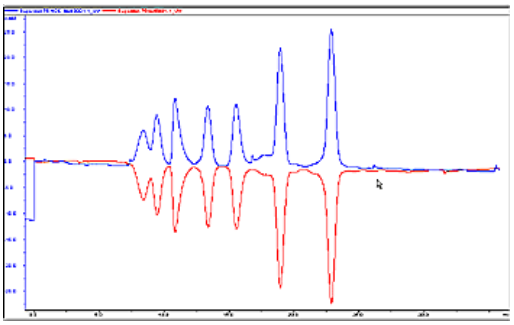
Stack



The curves are presented with a given offset Y-axis value so that the curves are stacked and distinct from one another.

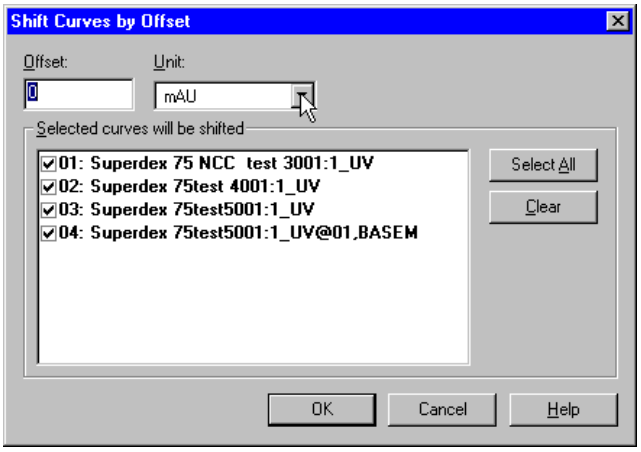
Step	Action

Mirror



For comparison of *two* imported curves. One curve is inverted in the Y-axis and thus appears to mirror the other curve.

5 If you selected the ***Stack*** option in step 3, the ***Shift Curves by Offset*** dialog box is displayed:



- You can set the ***Offset*** value to increase or decrease the offset distance between the curves.
- Click ***OK***.

Result: Depending on your previous choices, the imported curves are now displayed in the source chromatogram or in a newly created chromatogram.

Note: If curves with several different units have been selected, the curves with each different unit will be grouped together with separate offset from the other groups.

Step	Action
6	**Change some comparison settings** • Choose ***Edit:Chromatogram Layout*** to open the ***Chromatogram Layout*** dialog box. • Select or de-select the check boxes on the ***Curve*** tab to compare a different set of curves. • On the ***Y-Axis*** tab, the curves can be scaled - individually - all with the same scale (click the ***All with this unit*** button). • Click ***OK*** to display the curves.
7	If you stacked the curves and want to change the stack offset • choose ***Operations:Shift offset*** • type a new ***Offset*** value and click ***OK***. **Note:** The individual curves can also be moved (see *Section 11.8.4 How to stack and stretch curves, on page 380*).

How to use File:Open:Curves

The table below describes how to import individual curves into an active chromatogram with the ***File:Open:Curves*** command:

Step	Action
1	Make sure that the destination chromatogram for the imported curve(s) is active on the screen.
2	Select ***File:Open:Curves*** in the ***Evaluation*** module. *Result*: The ***Open Curves*** dialog box is displayed.

Step	Action
3	**Select curves in the Open curves dialog box** • Select the folder and the result file in the upper part of the dialog box. • Select a chromatogram on the ***Chromatogram*** drop-down list. Usually there is just one chromatogram. *Result*: The available curves are listed on the ***Available*** list. • Click the check boxes on the ***Available*** list for the curves that you want to import and click the ***Select*** button. *Result*: The selected curve(s) is displayed in the ***Selected curves*** list. To remove a curve from the ***Selected curves*** list, click the check box and then click the ***Remove*** button.
4	Click ***OK*** when you have selected the curves you want.
5	Repeat step 2 to 4 if you want to import curves from other chromatograms.
6	**Change some comparison settings** • Choose ***Edit:Chromatogram Layout*** to open the ***Chromatogram Layout*** dialog box. • Select or de-select the check boxes on the ***Curve*** tab to compare a different set of curves. • On the ***Y-Axis*** tab, the curves can be scaled - individually - all with the same scale (click the ***All with this unit*** button). • Click ***OK*** to display the curves.

How to copy curves into one chromatogram

A practical way to compare curves is to create a chromatogram and copy curves from different chromatograms into the new chromatogram. The comparisons are then performed in the new chromatogram.

The table below describes how to copy curves into a chromatogram:

Step	Action
1	Perform *either* A or B below: **A. Create a new chromatogram** • Choose ***File:New:Chromatogram*** to create a new chromatogram. **B. Use the Temporary chromatogram** • Choose ***Window:Temporary***.
2	**Open the source chromatogram(s)** Choose ***File:Open:Chromatogram*** to open the chromatogram(s) that contains the curves you want to copy. *Result*: The ***Open Chromatogram*** dialog box opens.
3	• Select the result file. • Click the check box for the source chromatogram in the ***Available*** list. • Click the ***Select*** button. • Click ***OK***. *Result*: The source chromatogram opens.
4	**Copy the curves** • Choose ***Edit:Copy:Curves***. *Result*: The ***Copy Curve*** dialog box is displayed.
5	• Select the source chromatogram and a curve of interest in the ***Source Chromatogram*** field. • Select the target chromatogram (the one you created, or ***Temporary***) in the ***Target Chromatogram*** field. • Click the ***Copy*** button. • Repeat this step for as many curves as you want, from the same or other chromatograms. **Note:** You can open more source chromatograms with the ***File:Open:Chromatogram*** command.
6	Click the ***Close*** button when you have copied all curves.

Step	Action
7	**Change some comparison settings** • Make sure the target chromatogram is open and that its window is active. • Choose ***Edit:Chromatogram Layout*** to display the ***Chromatogram Layout*** dialog box. • Select the curves that you want to view on the ***Curve*** tab and click ***OK***. • The curves can be scaled individually or all with the same Y-axis scale. Use the ***All with this unit*** button on the ***Y-Axis*** tab to scale all curves with the same scale.
8	**If you used the Temporary chromatogram** • If you used the ***Temporary*** chromatogram you can perform evaluations in the ***Temporary*** chromatogram and transfer the final curves to other destination chromatograms. • All of the contents in the ***Temporary*** chromatogram can be removed with ***Edit:Clear Temporary Chromatogram***.

Alternative way to copy curves

An alternative way to copy curves into one chromatogram is to

- create a new chromatogram by copying an existing chromatogram and saving it under a new name
- import more curves into the new chromatogram according to the instructions described above in this section.

11.8.4 How to stack and stretch curves

Functions

You can stack and stretch curves from different runs to better visualize the differences. To achieve this you can use the following functions:

- ***Normalize***
- ***Shift***
- ***Multiply***.

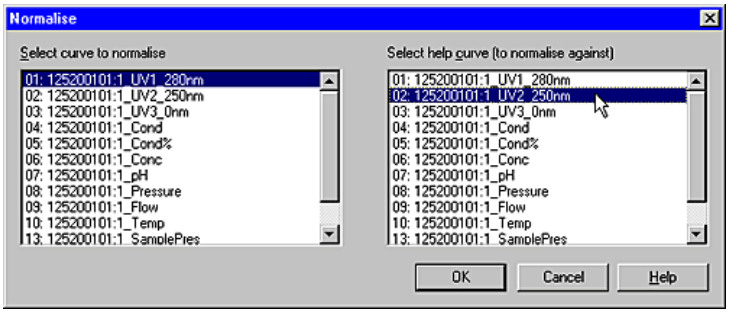
Note: All the functions require the curves to be present in one chromatogram.

How to use the Normalize function

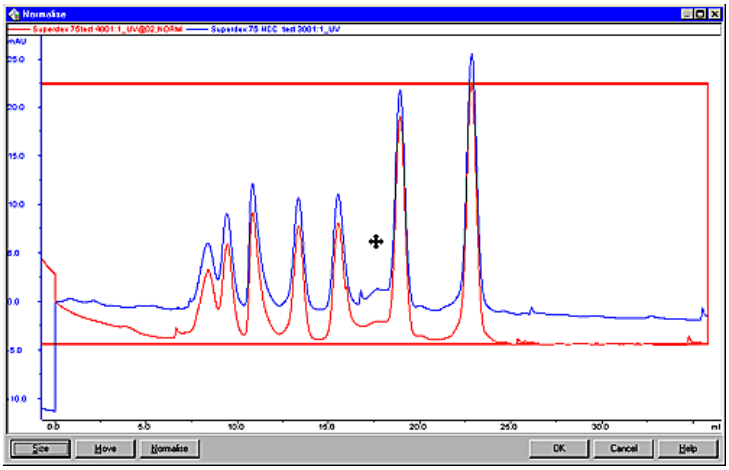
The ***Normalize*** function provides the simplest method to align curves with respect to the X-axis or the Y-axis for easier visualization.

The table below describes how to use the ***Normalise*** function:

Step	Action
1	• Make sure that a chromatogram with the relevant curves is open in the ***Evaluation*** module. • Choose ***Operations:Normalize***. *Result*: The ***Normalise*** dialog box is displayed.



Step	Action
2	• Select the curve you want to normalise in the left (***Select curve to normalise***) field. • Select the reference curve you want to normalise *against* in the right (***Select help curve***) field.*Example*: If you want to *stack* the curves, select the curve at the bottom of the stack as the reference curve. • Click ***OK***. *Result*: The ***Normalise*** window is displayed, where a box surrounds the curve selected to be normalised.



Step	Action
3	In the ***Normalise*** window, you can use the following command buttons: ***Size*** Allows the arrow keys to be used to stretch the selected curve along its Y-axis or X-axis. This is useful for comparison of curves with, for example, different gradient lengths. • Click the ***Size*** button and use the arrow keys to stretch the the curve either along its Y-axis or X-axis. ***Move*** Allows the arrow keys to be used to move the selected curve to any position on the chromatogram. Axes are automatically re-scaled to accommodate the new positioning. This function is useful for stacking curves. • Click the ***Move*** button and use the arrow keys to move the curve into position. The curve can also be moved with the mouse pointer. Click the mouse button when the curve is in the correct position. **Note:** The curve can also be moved and sized with the mouse pointer. ***Normalize*** The curve to be normalized will be adjusted to the help curve. Thus, the height of the highest peak on both curves will be the same and will occur at the same retention point. • Click the ***Normalize*** button. The curve to be normalized is automatically moved along the X-axis and stretched along the Y-axis. • Click ***OK*** to save the new normalised curve. *Result*: The ***Save Curve*** dialog box opens.
4	Choose a curve position to save the curve in and click ***OK***.
5	• Choose ***Edit:Chromatogram Layout*** to open the ***Chromatogram Layout*** dialog box. • Select the normalised curve for viewing on the ***Curve*** tab. • Click ***OK***.
6	Repeat steps 1-5 for all curves you want to stack or stretch.

How to move a curve with the Shift function

If you want to position a curve more precisely, the ***Shift*** function should be used. The function is similar to ***Normalize:Move*** but each curve is repositioned by a precise value instead of by eye and the instruction is logged in the evaluation log. The table below describes how to use the ***Shift*** function:

Step	Action
1	• Make sure that a chromatogram with the relevant curves is open in the ***Evaluation*** module. • Choose ***Operations:Shift***. *Result*: The ***Shift*** dialog box is displayed.
2	• Select the curve to be shifted in the ***Source chromatogram*** list. • Select a curve position in the ***Target chromatogram*** list. • Type a new ***Curve name*** or accept the default. • Select the axis/axes along which the shift is to be made: - along the X-axis (***Shift retention***) - along the Y-axis (***Shift amplitude***). • Type the shift value(s).
3	Click ***OK***.

How to stretch and shrink a curve with the Multiply function

Curves can be stretched or shrunk on the x or y plane with the ***Multiply*** function. This function is similar to ***Normalize:Size***, but each curve is repositioned with precise numbers instead of by eye and the instruction logged in the evaluation log. The table below describes how to use the ***Multiply*** function:

Step	Action
1	• Make sure that a chromatogram with the relevant curves is open in the ***Evaluation*** module. • Choose ***Operations:Multiply***. *Result*: The ***Multiply*** dialog box is displayed.

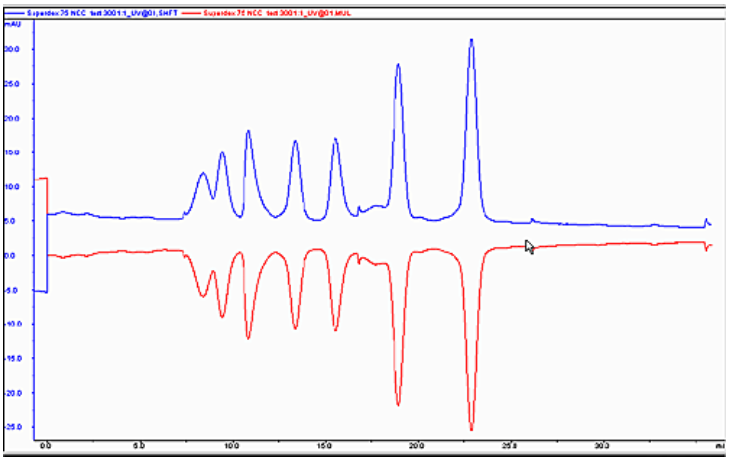
Step	Action
2	• Select the curve to be multiplied in the ***Source chromatogram*** list. • Select a curve position in the ***Target chromatogram*** list. • Type a new ***Curve name*** or accept the default. • Select the axis/axes along which the multiplication is to be made: - along the X-axis (***Multiply retention***) - along the Y-axis (***Multiply amplitude***). • Type the multiply value(s).
3	Click ***OK***.

11.8.5 How to produce a mirror image

Instruction

A very useful way to compare the features of two curves is to produce a mirror image of one curve. The table below describes how to do this:

Step	Action
1	• Make sure that a chromatogram with the relevant curves is open in the ***Evaluation*** module. • Choose ***Operations:Multiply***. *Result*: The ***Multiply*** dialog box is displayed.
2	• Select the curve to be multiplied in the ***Source chromatogram*** list. • Select a curve position in the ***Target chromatogram*** list. • Type a new ***Curve name*** or accept the default. • Select the ***Multiply amplitude*** check box. • Type the multiply value `-1`. • Click ***OK***. *Result*: The mirror image of the original curve is displayed in the active chromatogram window.

Step	Action
3	**Shift the mirror image curve downwards** Shift the mirror image curve downwards for an improved presentation: • Choose ***Operations:Shift***. *Result*: The ***Shift*** dialog box is displayed. • Select the curve to be shifted in the ***Source chromatogram*** list. • Select the same curve number in the ***Target chromatogram*** list box as in step 2. • Select the Shift amplitude check box since the shift is to be made along the Y-axis. • Type a shift value. • Click ***OK***. The illustration below shows the original curve and the mirror image displayed. 
4	If you want to display other curves in the active chromatogram window, • choose ***Edit:Chromatogram Layout*** to open the ***Chromatogram Layout*** dialog box • select the curves that you want to display • click ***OK***.

11.9 How to import and export results

Introduction

Curves and data can be imported and exported in different formats. This section describes how to import and export results.

In this section

This section contains these topics:

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11.9.1 How to import results

Introduction

This section describes how to import curves in different formats and how to import result data from ***SMART Manager*** or ***FPLCdirector™***.

Curve formats

You can import curve files in the following formats:

- AIA (.cdf)
- ASCII (text)
- Lotus 1-2-3 spreadsheet (.wks)

How to import curves

The table below describes how to import curves.

Step	Action
1	Choose ***File:Import:Curve***. *Result*: A menu with the available curve formats opens.
2	Choose the correct curve format. *Result*: The ***Choose File to Import From*** dialog box opens.
3	Locate the file that contains the curve and double-click the file. *Result*: The ***Import Curves*** dialog box opens.
4	Select the curve(s) to import and click the ***OK*** button. *Result*: The curves are opened in the ***Evaluation*** module.

How to import data from SMART Manager and FPLCdirector

The table below describes how to import data from ***SMART Manager*** and ***FPLCdirector***:

Step	Action
1	Choose ***File:Import:Result***. *Result*: A menu box with the available data sources opens. This box opens immediately after ***Import*** if no result file is open in the ***Evaluation*** module.
2	Choose ***FPLCdirector*** or ***SMART***. *Result*: The ***Import FPLCdirector Result*** dialog box or the ***Import SMART Result*** dialog box opens.
3	Locate and double-click the result file. *Result*: The result file is opened in the ***Evaluation*** module.

Copy from a floppy disk

When you import ***SMART*** or ***FPLCdirector*** files from a floppy disk it is best to first copy the files to the hard disk and then import the files.

11.9.2 How to export results

Introduction

This section describes how to export curves in different formats and how to copy data and curves to the clipboard.

Data formats

You can export data in the following formats:

- AIA (.cdf)
- ASCII (.asc)
- Lotus 1-2-3 (.wks)
- Excel (.xls)
- XML (.xml)

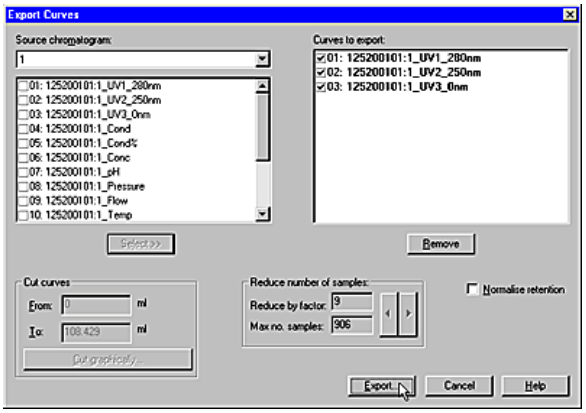
Export options

Select ***File:Export*** in the ***Evaluation*** module to export data from an open result file. The following export options are available:

- ***Curves***
- ***Export curve to AIA***
- ***Peak table***
- ***Method***
- ***Documentation***
- ***Evaluation log***

How to export curves

The table below describes how to export curves in the ***Evaluation*** module.

Step	Action
1	Choose ***File:Export:Curves***. *Result*: The ***Export Curves*** dialog box opens.  Export Curves Source chromatogram: 1 01: 1252001101:1_UV1_280nm 02: 1252001101:1_UV2_250nm 03: 1252001101:1_UV3_0nm 04: 1252001101:1_Cond 05: 1252001101:1_Cond% 06: 1252001101:1_Conc 07: 1252001101:1_pH 08: 1252001101:1_Pressure 09: 1252001101:1_Flow 10: 1252001101:1_Temp Curves to export: 01: 1252001101:1_UV1_280nm 02: 1252001101:1_UV2_250nm 03: 1252001101:1_UV3_0nm Select >>>>

Note: Curves are exported as series of numerical coordinates that refers to the time/volume and signal respectively.

How to limit the exported curves

You can optimize the exported curves to only the parts that you want to focus on, in the ***Export Curves*** dialog box. The table below describes how to use these editing options.

Dialog box option	Instruction
Cut curves	Enter retention values in the text boxes to limit the curve to only a portion of the original curve.
Cut graphically	This button opens the ***Export Cut*** dialog box. Move the vertical markers to the correct cutoff points.
Reduce number of samples	Adjust the factor value or the maximum number of samples. To reduce the number of samples by a factor of five means that only every fifth point will be sampled for export.
Normalize retention	Select the ***Normalize retention*** checkbox to have all exported curves normalized to a common X-axis.

How to export curves in AIA format

The table below describes how to export curves in AIA format.

Step	Action
1	Select ***File:Export:Export curve to AIA***. *Result*: The ***Export curve in AIA format*** dialog box opens.
2	• Select the source chromatogram and the curve you want to export. • Click the ***Export*** button. *Result*: The ***Export Curves to File*** dialog box opens.
3	• Select a destination folder. • Type a file name. • Click ***OK***.

How to export peak tables

The table below describes how to export peak tables.

Step	Action
1	Choose ***File:Export:Peak Table***. *Result*: The ***Export Peak Table*** dialog box opens.
2	• Select the source chromatogram and the peak table you want to export. • Click the ***Export*** button. *Result*: The ***Export Peak Table to File*** dialog box opens.
3	Select the export file format from the ***Save as type*** drop-list. • ***ASCII files (*.asc)*** • ***Lotus 1-2-3 files (*.wks)*** • ***Excel files (*.xls)*** • ***XML files (*.xml)***
4	• Select a destination folder. • Type a file name. • Click ***OK***.

Note: Peak tables are exported as text strings in ASCII format and numerical values in the Lotus 1-2-3 formats. All possible columns in the peak table are exported.

How to export methods, documentation and evaluation logs

The table below shows how to export methods, documentation and evaluation logs:

Step	Action
1	Select the data you want to export.
2	• Select options in the dialog box. • Click the ***Export*** button.

Step	Action
3	• Select a destination folder and type a file name. • Click ***OK***.

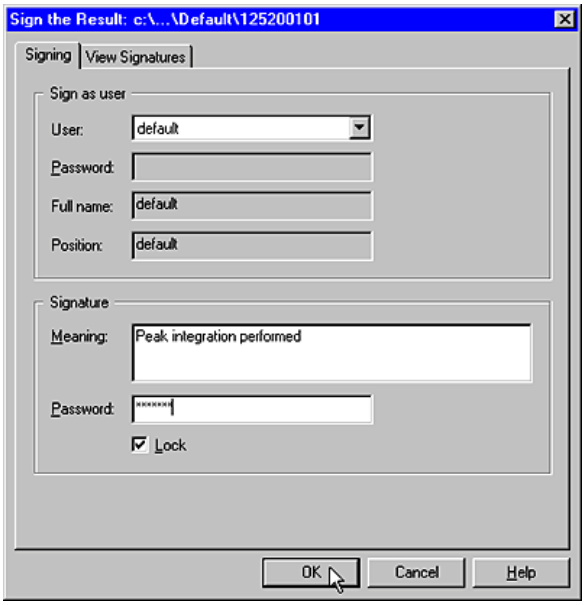
Copy to the clipboard

You can also use the ***Windows*** clipboard to copy the contents of the active window and paste it into other programs, e.g. ***Microsoft Word***. Curves and documentation are copied as Windows enhanced metafiles (.emf) and peak tables are copied as text. Only the peak table columns that are selected in the spreadsheet will be copied.

1110 How to sign results electronically

Instruction

Result files can be signed electronically to enhance data file security. The table below describes how to sign a result file electronically in the ***Evaluation*** module:

Step	Action
1	Choose ***File:Sign Result***. *Result*: The ***Sign the Result*** dialog box opens. 
2	• The ***Sign as user*** field shows the properties for the current user. You can also choose another user from the droplist. If you choose a new user, the corresponding password must be typed in the ***Password*** text box. • Type a short text description for the signed operation in the ***Meaning*** field (e.g. Peak integration performed). • The ***Lock*** check box is selected as default, to lock the result file from further changes. • Type your signature password in the ***Password*** field and click ***OK***. **Note:** You should only lock the result when you are sure that the result file will not be modified anymore.

Signatures associated with the result

The ***View Signatures*** tab of the ***Sign the Result*** dialog box provides a list of all signatures associated with the current result. The information on this tab is for viewing purposes only and cannot be changed.

1111 How to save results and exit the Evaluation module

Introduction

After you have finished the evaluation process, you can save all the changes you have made to the chromatograms, including newly created curves and chromatograms that you have imported and created.

How to delete unwanted curves

All the curves that you created during your manipulations will be saved in the chromatogram. If some of these curves are not be needed anymore, select ***Edit:Delete:Curves*** in the ***Evaluation*** module to remove the curves.

Note: The original curves that were created during the run can never be deleted.

How to save the results

You can either save your edited results in the original file or in a new result file. The table below describes how to save the results in the ***Evaluation*** module.

If you want to save the edited results...	then...
in the original result file	• select ***File:Save***. *or* • click the ***Save*** toolbar icon.
in a new result file	select ***File:Save as***.

Note: The previous version of the result file will be overwritten if you save the changes. This cannot be reversed. However, the raw data curves remain unchanged.

How to exit the Evaluation module

The table below describes how to exit the ***Evaluation*** module:

Step	Action
1	Choose ***File:Exit***. *Result*: If there are unsaved changes, a dialog box opens with an option to save the changes before exit.
2	Select ***Yes*** if you want to save the changes. *Result*: The result file is closed in the ***Evaluation*** module and the ***UNICORN Manager*** module is displayed.

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